

# THE HAHN POLYNOMIALS IN THE NONRELATIVISTIC AND RELATIVISTIC COULOMB PROBLEMS

SERGEI K. SUSLOV AND BENJAMIN TREY

*Dedicated to the memory of Arnold F. Nikiforov and Vasilii B. Uvarov*

**ABSTRACT.** We derive closed formulas for mean values of all powers of  $r$  in nonrelativistic and relativistic Coulomb problems in terms of the Hahn and Chebyshev polynomials of a discrete variable. A short review on special functions and solution of the Coulomb problems in quantum mechanics is given.

## 1. INTRODUCTION

A basic problem in quantum theory of the atom is the problem of finding solutions of the non-relativistic Schrödinger and relativistic Dirac wave equations for the motion of electron in a central attractive force field. The only atom for which these equations can be solved explicitly is the simplest hydrogen atom, or, in general, the one electron hydrogen-like ionized atom with the charge of the nucleus  $Ze$ ; this is a classical problem in quantum mechanics which is studied in great detail; see, for example, [1], [17], [16], [29], [39], [47], [51], [54], [64] and references therein. Comparison of the results of theoretical calculations with experimental data provides accurate tests of the validity of the quantum electrodynamics [17], [47], [82]. Explicit analytical solutions for hydrogen-like atoms can be useful as the starting point in approximate calculations of more sophisticated quantum-mechanical systems.

The Schrödinger equation for the hydrogen atom can be solved explicitly in the spherical and parabolic system of coordinates [17], [51] and it can be shown that the Hahn polynomials connect the wave functions derived in the spherical and parabolic coordinates; see [70] and references therein for more details. In the present paper we discuss another connection with the classical polynomials — we derive closed formulas for the mean values

$$\langle r^p \rangle = \int_{\mathbf{R}^3} \psi^\dagger r^p \psi \, dv \quad (1.1)$$

of all admissible powers of  $r$  for both nonrelativistic and relativistic Coulomb wave functions in the spherical coordinates in terms of the Hahn and Chebyshev polynomials of a discrete variable; see, for example, [2], [3], [4], [5], [6], [7], [8], [36], [42], [48], [49], [55], [56], [57], [74], and [75], [76], [77] for an introduction to the theory of the classical orthogonal polynomials. Special cases  $p = 0, 1, 2$  of (1.1) give the normalization of the wave functions, the average distance between the electron and

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the nucleus, and the mean square deviation of the nucleus-electron separation, respectively. Special cases  $p = -1, -2, -3$  of these matrix elements are important in calculations of the energy levels by the virial theorem, the fine structure of the energy levels in Pauli's theory of the spin, radiative corrections and Lamb shift in hydrogen-like atoms; see [1], [17], [16], [47], [51], [54], [82] for more details. The general formulas for the corresponding relativistic Coulomb matrix elements may also be important in developing the theory of spectra of heavy ions for large values of  $Z$  on the basis of the methods of quantum field theory [19], [20], [78].

It is worth noting that exact solutions of certain time-dependent Schrödinger equations are found in [52] and [53]. An interesting area of research in physics in general is a problem of discretization of the space-time continuum and the concept of the fundamental length [46], [60] and, in particular, the discretization of the classical Maxwell, Schrödinger and Dirac equations; see [37] and [72] for some solutions of the discrete wave, Maxwell and Dirac equations.

The paper is organized as follows. In the next section, among other things, we evaluate an integral of the product of two Laguerre polynomials in terms of the Hahn polynomials, which gives a “master formula” for evaluation of the matrix elements (1.1) for the nonrelativistic and relativistic hydrogen-like atoms in sections 3 and 4, respectively. Some special cases are given explicitly and evaluation of the effective electrostatic potential in the hydrogen-like atoms is discussed as an application. Sections 5 and 6 are written in order to make our presentation as self-contained as possible — they contain a short review of Nikiforov and Uvarov's approach to the theory of special functions of mathematical physics and a detailed solution of the wave equation of Dirac for Coulomb potential, respectively. We follow [57] with somewhat different details; for example, in Section 5 we give a different proof of the main integral representation for the special functions of hypergeometric type and discuss the power series method; in Section 6 we construct the spinor spherical harmonics and separate the variables in the spherical coordinates in detail before solving the radial equations. In Section 7 we discuss a more general version of the method of separation of the variables for Dirac-type systems. The relativistic Coulomb wave functions are not well known for a “general audience” and this discussion might be useful for the reader who is not an expert in theoretical physics; our paper is written for those who study quantum mechanics and would like to see more details than in the classical textbooks [1], [17], [16], [51]; it is motivated by a course in quantum mechanics which one of the authors (SKS) has been teaching at Arizona State University for many years. Appendix contains some formulas which are widely used throughout the paper.

We use the absolute cgs system of units throughout the paper in order to make the corresponding nonrelativistic limits as explicit as possible. The fundamental constants are speed of light in vacuum  $c = 2.99792458 \times 10^{10}$  cm s $^{-1}$ , Planck's constant  $\hbar = 6.6260755 \times 10^{-34}$  J s, mass  $m = m_e = 9.1093897 \times 10^{-28}$  gm and electric charge  $e = |e| = 1.60217733 \times 10^{-19}$  C of the electron, Bohr radius  $a_0 = \hbar^2/me^2 = 0.529177249 \times 10^{-8}$  cm, Sommerfeld's fine structure constant  $\alpha = e^2/\hbar c = 7.29735308 \times 10^{-3}$ , and Compton wave length  $\lambda/2\pi = \hbar/mc = 2.42631058 \times 10^{-10}$  cm.

We dedicate this paper to the memory of Professors A. F. Nikiforov and V. B. Uvarov in a hope that those masters would appreciate our effort to make their method more available for the beginners.

## 2. SOME INTEGRALS OF THE PRODUCTS OF LAGUERRE POLYNOMIALS

**2.1. Evaluation of an Integral.** Let us compute the following integral

$$J_{nms}^{\alpha\beta} = \int_0^\infty e^{-x} x^{\alpha+s} L_n^\alpha(x) L_m^\beta(x) dx, \quad (2.1)$$

where  $n \geq m$  and  $\alpha - \beta = 0, \pm 1, \pm 2, \dots$ . Similar integrals were evaluated in [17], [28] and [51], see also references therein, but an important relation with the Hahn polynomials seems to be missing.

It is convenient to assume at the beginning that parameter  $s$  takes some continuous values such that  $\alpha + s > -1$  for convergence of the integral. Using the Rodrigues formula for the Laguerre polynomials [55], [57], [74]

$$L_n^\alpha(x) = \frac{1}{n!} e^x x^{-\alpha} (x^{\alpha+n} e^{-x})^{(n)}, \quad (2.2)$$

see the proof in Section 5 of the present paper, and integrating by parts

$$\begin{aligned} J_{nms}^{\alpha\beta} &= \frac{1}{n!} \int_0^\infty (x^{\alpha+n} e^{-x})^{(n)} (x^s L_m^\beta(x)) dx \\ &= \frac{1}{n!} \left( (x^{\alpha+n} e^{-x})^{(n-1)} (x^s L_m^\beta(x)) \right) \Big|_0^\infty - \frac{1}{n!} \int_0^\infty (x^{\alpha+n} e^{-x})^{(n-1)} (x^s L_m^\beta(x))' dx \\ &\quad \vdots \\ &= \frac{(-1)^n}{n!} \int_0^\infty (x^{\alpha+n} e^{-x}) (x^s L_m^\beta(x))^{(n)} dx. \end{aligned}$$

But, in view of (8.2),

$$\begin{aligned} (x^s L_m^\beta(x))^{(n)} &= \frac{\Gamma(\beta + m + 1)}{m! \Gamma(\beta + 1)} \sum_k \frac{(-m)_k}{k! (\beta + 1)_k} (x^{k+s})^{(n)} \\ &= \frac{\Gamma(\beta + m + 1) \Gamma(s + 1)}{m! \Gamma(\beta + 1) \Gamma(s - n + 1)} \sum_k \frac{(-m)_k (s + 1)_k}{k! (\beta + 1)_k (s - n + 1)_k} x^{k+s-n} \end{aligned} \quad (2.3)$$

and with the help of Euler's integral representation for the gamma function [3], [57]

$$\int_0^\infty x^{\alpha+k+s} e^{-x} dx = \Gamma(\alpha + k + s + 1) = (\alpha + s + 1)_k \Gamma(\alpha + s + 1),$$

see also (8.11) below, one gets

$$\begin{aligned} J_{nms}^{\alpha\beta} &= (-1)^n \frac{\Gamma(\alpha + s + 1) \Gamma(\beta + m + 1) \Gamma(s + 1)}{n! m! \Gamma(\beta + 1) \Gamma(s - n + 1)} \\ &\quad \times {}_3F_2 \left( \begin{matrix} -m, s + 1, \alpha + s + 1 \\ \beta + 1, s - n + 1 \end{matrix} \right). \end{aligned} \quad (2.4)$$

See [10] or equation (8.1) below for the definition of the generalized hypergeometric series  ${}_3F_2(1)$ . Thomae's transformation (8.9), see also [10] or [42], results in

$$\begin{aligned} J_{nms}^{\alpha\beta} &= \int_0^\infty e^{-x} x^{\alpha+s} L_n^\alpha(x) L_m^\beta(x) dx \\ &= (-1)^{n-m} \frac{\Gamma(\alpha + s + 1) \Gamma(\beta + m + 1) \Gamma(s + 1)}{m! (n - m)! \Gamma(\beta + 1) \Gamma(s - n + m + 1)} \end{aligned} \quad (2.5)$$

$$\times {}_3F_2 \left( \begin{matrix} -m, s+1, \beta - \alpha - s \\ \beta + 1, n - m + 1 \end{matrix} \right), \quad n \geq m,$$

where parameter  $s$  may take some integer values. This establishes a connection with the Hahn polynomials given by equation (8.7) below; one can also rewrite this integral in terms of the dual Hahn polynomials [55].

**2.2. Special Cases.** Letting  $s = 0$  and  $\alpha = \beta$  in (2.5) results in the orthogonality relation for the Laguerre polynomials. Two special cases

$$I_1 = J_{nn1}^{\alpha\alpha} = \int_0^\infty e^{-x} x^{\alpha+1} (L_n^\alpha(x))^2 dx = (\alpha + 2n + 1) \frac{\Gamma(\alpha + n + 1)}{n!} \quad (2.6)$$

and

$$I_2 = J_{n, n-1, 2}^{\alpha-2, \alpha} = \int_0^\infty e^{-x} x^\alpha L_{n-1}^\alpha(x) L_n^{\alpha-2}(x) dx = -2 \frac{\Gamma(\alpha + n)}{(n-1)!} \quad (2.7)$$

are convenient for normalization of the wave functions of the discrete spectra in the nonrelativistic and relativistic Coulomb problems [17], [57].

Two other special cases of a particular interest in this paper are

$$\begin{aligned} J_k &= J_{nnk}^{\alpha\alpha} = \int_0^\infty e^{-x} x^{\alpha+k} (L_n^\alpha(x))^2 dx \\ &= \frac{\Gamma(\alpha + k + 1) \Gamma(\alpha + n + 1)}{n! \Gamma(\alpha + 1)} {}_3F_2 \left( \begin{matrix} -k, k+1, -n \\ 1, \alpha+1 \end{matrix} \right) \end{aligned} \quad (2.8)$$

and

$$\begin{aligned} J_{-k-1} &= J_{nn, -k-1}^{\alpha\alpha} = \int_0^\infty e^{-x} x^{\alpha-k-1} (L_n^\alpha(x))^2 dx \\ &= \frac{\Gamma(\alpha - k) \Gamma(\alpha + n + 1)}{n! \Gamma(\alpha + 1)} {}_3F_2 \left( \begin{matrix} -k, k+1, -n \\ 1, \alpha+1 \end{matrix} \right). \end{aligned} \quad (2.9)$$

The Chebyshev polynomials of a discrete variable  $t_k(x)$  are special case of the Hahn polynomials  $t_k(x, N) = h_k^{(0, 0)}(x, N)$  [75], [76] and [77]. Thus from (2.8)–(2.9) and (8.7) one finally gets

$$\begin{aligned} J_k &= J_{nnk}^{\alpha\alpha} = \int_0^\infty e^{-x} x^{\alpha+k} (L_n^\alpha(x))^2 dx \\ &= \frac{\Gamma(\alpha + n + 1)}{n!} t_k(n, -\alpha) \end{aligned} \quad (2.10)$$

and

$$\begin{aligned} J_{-k-1} &= J_{nn, -k-1}^{\alpha\alpha} = \int_0^\infty e^{-x} x^{\alpha-k-1} (L_n^\alpha(x))^2 dx \\ &= \frac{\Gamma(\alpha - k) \Gamma(\alpha + n + 1)}{n! \Gamma(\alpha + k + 1)} t_k(n, -\alpha) \end{aligned} \quad (2.11)$$

for  $0 \leq k < \alpha$ . One can see that the positivity of these integrals is related to a nonstandard orthogonality relation for the corresponding Chebyshev polynomials of a discrete variable  $t_k(x, N)$  when the parameter takes negative integer values  $N = -\alpha$ . Indeed, according to the method of [55]

and [57], these polynomials are orthogonal with the discrete uniform distribution on the interval  $[-\alpha, -1]$  which contains all their zeros and, therefore, they are positive for all nonnegative values of their argument. The explicit representation (8.7) gives also a positive sum for all positive  $x$  and negative  $N$ .

**2.3. Connection Relation and Linearization Formula.** The connection relation [3], [4]

$$L_n^\alpha(x) = \sum_{m=0}^n \frac{(\alpha - \beta)_{n-m}}{(n-m)!} L_m^\beta(x) \quad (2.12)$$

is an easy consequence of the integral (2.5), we leave the details to the reader.

A linearization formula

$$L_n^\alpha(x) L_m^\beta(x) = \sum_{p=0}^{n+m} c_{nmp}(\alpha, \beta, \gamma) L_p^\gamma(x) \quad (2.13)$$

gives a product of two Laguerre polynomials as a linear combination of other polynomials of the same kind; see [3], [4], [7], [61], [62] and references therein for a review on the linearization of products of classical orthogonal polynomials. In view of the orthogonality relation, the corresponding linearization coefficients are given by

$$\frac{\Gamma(\gamma + p + 1)}{p!} c_{nmp}(\alpha, \beta, \gamma) = \int_0^\infty L_n^\alpha(x) L_m^\beta(x) L_p^\gamma(x) x^\gamma e^{-x} dx, \quad (2.14)$$

where one can assume that  $n \geq m$  and use the expansion

$$L_p^\gamma(x) = \frac{\Gamma(\gamma + p + 1)}{p! \Gamma(\gamma + 1)} \sum_{k=0}^p \frac{(-p)_k}{k! (\gamma + 1)_k} x^k \quad (2.15)$$

by (8.2). Then the integral of the product of three Laguerre polynomials is

$$\begin{aligned} c_{nmp}(\alpha, \beta, \gamma) &= \frac{1}{\Gamma(\gamma + 1)} \sum_{k=0}^p \frac{(-p)_k}{k! (\gamma + 1)_k} \int_0^\infty e^{-x} x^{\gamma+k} L_n^\alpha(x) L_m^\beta(x) dx \\ &= \frac{1}{\Gamma(\gamma + 1)} \sum_{k=0}^p \frac{(-p)_k}{k! (\gamma + 1)_k} J_{nm, \gamma-\alpha+k}^{\alpha\beta} \end{aligned} \quad (2.16)$$

and the remaining integral can be evaluated in terms of the Hahn or dual Hahn polynomials with the aid of (2.5). Positivity of the linearization coefficients is related to the orthogonality property of these polynomials.

On the other hand, in the most important special case,

$$L_n^\alpha(x) L_m^\alpha(x) = \sum_{p=n-m \geq 0}^{n+m} c_{nmp} L_p^\alpha(x) \quad (2.17)$$

with  $\alpha = \beta = \gamma$ , the linearization coefficients  $c_{nmp}(\alpha) = c_{nmp}(\alpha, \alpha, \alpha)$  can be found as a single sum

$$c_{nmp} = (-1)^p \frac{(-p)_{n-m} (\alpha + 1)_m}{p! m!} \sum_k \frac{(-p)_k (-m)_k \Gamma(2k + 1)}{k! (\alpha + 1)_k \Gamma(n - m - p + 2k + 1)}. \quad (2.18)$$

The summation is to be taken over all integer values of  $k$  such that  $0 \leq p - n + m \leq 2k \leq \min(2p, 2m)$ .

Indeed, substituting (2.5) into (2.16)

$$\begin{aligned} \Gamma(\alpha + 1) c_{nmp} &= (-1)^{n-m} \frac{\Gamma(\alpha + m + 1)}{m! (n - m)!} \sum_{s=n-m \geq 0}^p \frac{(-p)_s}{\Gamma(s - n + m + 1)} \\ &\times \sum_{k=0}^{\min(m,s)} \frac{(-m)_k (-s)_k (s+1)_k}{k! (\alpha + 1)_k (n - m + 1)_k} \end{aligned} \quad (2.19)$$

with  $\alpha = \beta = \gamma$ , then replacing the index  $s = n - m + l$ ,  $0 \leq l \leq p - n + m$  and changing the order of summation one gets

$$\begin{aligned} \Gamma(\alpha + 1) c_{nmp} &= (-1)^{n-m} \frac{\Gamma(\alpha + m + 1)}{m! (n - m)!} (-p)_{n-m} \\ &\times \sum_k \frac{(-m)_k (-n + m)_k}{k! (\alpha + 1)_k} \\ &\times \sum_l \frac{(-p + n - m)_l (n - m + k + 1)_l}{l! (n - m - k + 1)_l} \end{aligned} \quad (2.20)$$

with the help of

$$\begin{aligned} (-p)_{n-m+l} &= (-p)_{n-m} (-p + n - m)_l, \\ (-n + m - l)_k &= (-n + m)_k \frac{(n - m + 1)_l}{(n - m - k + 1)_l}, \\ (n - m + l + 1)_k &= (n - m + 1)_k \frac{(n - m + k + 1)_l}{(n - m + 1)_l}. \end{aligned}$$

The  ${}_2F_1(1)$  function in (2.20) is evaluated by a limiting case of the Gauss summation formula (8.10) as

$$\begin{aligned} (-n + m)_k {}_2F_1 \left( \begin{matrix} -p + n - m, n - m + k + 1 \\ n - m - k + 1 \end{matrix} ; 1 \right) \\ = (-1)^{n-m-p} (-p)_k \frac{(n - m)! \Gamma(2k + 1)}{p! \Gamma(n - m - p + 2k + 1)}. \end{aligned} \quad (2.21)$$

This results in (2.18) and our proof is complete.

Equations (2.14) and (2.18) imply the following positivity property

$$(-1)^{m+n+p} \int_0^\infty L_n^\alpha(x) L_m^\alpha(x) L_p^\alpha(x) x^\alpha e^{-x} dx \geq 0, \quad (2.22)$$

when  $\alpha > -1$  and  $m, n, p = 0, 1, 2, \dots$ ; see problem 33 on p. 400 of [3].

The single sum in (2.18) can be rewritten as a  ${}_4F_3$ . There are distinct representations for even and odd values of  $\epsilon = (p - n + m)/2$ . When  $\epsilon = 0$  the summation formula (8.10) gives

$$c_{nm, n-m}(\alpha) = \frac{\Gamma(\alpha + n + 1)}{m! \Gamma(\alpha + n - m + 1)} \quad (2.23)$$

and the case  $n = m$  corresponds to correct value of the squared norm of the Laguerre polynomials. If  $\epsilon = (p - n + m) / 2$  is a positive even number the result is

$$\begin{aligned} c_{nmp}(\alpha) &= (-1)^p \frac{(-p)_{n-m} (-p)_\epsilon (-m)_\epsilon}{p! m!} \frac{\Gamma(2\epsilon + 1) \Gamma(\alpha + m + 1)}{\Gamma(\epsilon) \Gamma(\alpha + \epsilon + 1)} \\ &\quad \times {}_4F_3 \left( \begin{matrix} -p + \epsilon, -m + \epsilon, \epsilon + 1/2, \epsilon + 1 \\ 1/2, \alpha + \epsilon + 1, \epsilon \end{matrix} \right) \end{aligned} \quad (2.24)$$

and

$$\begin{aligned} c_{nmp}(\alpha) &= (-1)^p \frac{(-p)_{n-m} (-p)_{\epsilon+1/2} (-m)_{\epsilon+1/2}}{p! m!} \frac{\Gamma(2\epsilon + 2) \Gamma(\alpha + m + 1)}{\Gamma(\epsilon + 1/2) \Gamma(\alpha + \epsilon + 3/2)} \\ &\quad \times {}_4F_3 \left( \begin{matrix} -p + \epsilon + 1/2, -m + \epsilon + 1/2, \epsilon + 1, \epsilon + 3/2 \\ 3/2, \alpha + \epsilon + 3/2, \epsilon + 1/2 \end{matrix} \right), \end{aligned} \quad (2.25)$$

if  $\epsilon = (p - n + m) / 2$  is an odd.

Although we have not been able to find the linearization formula for Laguerre polynomials in explicit form in the literature, a closed expression for the linearization coefficients should follow as a limiting case of equations (1.7)–(1.8) for the linearization coefficients of the Jacobi polynomials in Rahman's paper [61]; see also [62] for  $q$ -extension of his result. Dick Askey has told us that he had computed the corresponding integral of the product of three Laguerre polynomials with the help of the generating function for these polynomials as a different single sum. In his opinion, this may have been found in the 1930's by Erdelyi or someone else.

**2.4. An Extension.** The integral (2.1) has a somewhat useful extension

$$J_{nms}^{\alpha\beta}(z) = \int_z^\infty e^{-x} x^{\alpha+s} L_n^\alpha(x) L_m^\beta(x) dx, \quad (2.26)$$

where  $n \geq m$  and  $\alpha - \beta = 0, \pm 1, \pm 2, \dots$  and  $J_{nms}^{\alpha\beta}(0) = J_{nms}^{\alpha\beta}$ . This integral is evaluated in the following fashion. Upon integrating by parts

$$\begin{aligned} J_{nms}^{\alpha\beta}(z) &= e^{-z} \sum_{k=1}^l (-1)^k \frac{(n-k)!}{n!} z^{\alpha+k} L_{n-k}^{\alpha+k}(z) (z^s L_m^\beta(z))^{(k-1)} \\ &\quad + \frac{(-1)^l}{n!} \int_z^\infty (x^{\alpha+n} e^{-x})^{(n-l)} (x^s L_m^\beta(x))^{(l)} dx \end{aligned} \quad (2.27)$$

and putting  $l = n$  we use (2.3) and the integral representation for incomplete gamma function [36], [57]:

$$\Gamma(\alpha, z) = \int_z^\infty e^{-x} x^{\alpha-1} dx, \quad \operatorname{Re} \alpha > 0. \quad (2.28)$$

As a result

$$\begin{aligned} J_{nms}^{\alpha\beta}(z) &= \int_z^\infty e^{-x} x^{\alpha+s} L_n^\alpha(x) L_m^\beta(x) dx \\ &= z^\alpha e^{-z} \sum_{k=1}^n (-1)^k \frac{(n-k)!}{n!} z^k L_{n-k}^{\alpha+k}(z) (z^s L_m^\beta(z))^{(k-1)} \end{aligned} \quad (2.29)$$

$$+ (-1)^n \frac{(\beta+1)_m}{n! m!} \sum_{k=0}^m \frac{(-m)_k \Gamma(s+k+1)}{k! (\beta+1)_k \Gamma(s-n+k+1)} \Gamma(\alpha+k+s+1, z)$$

with  $n \geq m$  and  $\operatorname{Re}(\alpha+s) > -1$ . Here one can use the standard relations [36], [57]:

$$\begin{aligned} \Gamma(\alpha, z) &= e^{-z} G(1-\alpha, 1-\alpha, z) \\ &= \Gamma(\alpha) - \frac{1}{\alpha} z^\alpha F(\alpha, 1+\alpha, -z) \\ &= \Gamma(\alpha) - z^\alpha \sum_{k=0}^{\infty} \frac{(-1)^k z^k}{k! (\alpha+k)}, \quad \operatorname{Re} \alpha > 0 \end{aligned} \tag{2.30}$$

with the confluent hypergeometric functions  $F(\alpha, \gamma, z)$  and  $G(\alpha, \gamma, z)$ , respectively. The last expression gives the asymptotic of the incomplete gamma function as  $z \rightarrow 0$  and  $|\arg(z)| < \pi$ . The asymptotic for large values of  $z$  is

$$\begin{aligned} \Gamma(\alpha, z) &= e^{-z} z^\alpha G(1, 1+\alpha, z) \\ &= e^{-z} z^{\alpha-1} \left( \sum_{k=0}^{n-1} (-1)^k \frac{(1-\alpha)_k}{z^k} + O\left(\frac{1}{z^n}\right) \right) \end{aligned} \tag{2.31}$$

as  $z \rightarrow \infty$  and  $|\arg(z)| < \pi$ ; see [36] and [57]. This allows to find asymptotic expansions of the integral (2.29) as  $z \rightarrow 0$  and  $z \rightarrow \infty$ . Integration by parts in (2.28) results in the functional relation

$$\Gamma(\alpha+1, z) = \alpha \Gamma(\alpha, z) + z^{\alpha-1} e^{-z}, \tag{2.32}$$

which implies

$$\Gamma(n+1, z) = n! e^{-z} \sum_{k=0}^n \frac{z^k}{k!} \tag{2.33}$$

for positive integers  $n$ .

### 3. NONRELATIVISTIC COLOUMB PROBLEM

**3.1. Wave Functions and Energy Levels.** The nonrelativistic Coulomb wave functions obtained by the method of separation of the variables in spherical coordinates, see Section 7.1, are

$$\psi = \psi_{nlm}(\mathbf{r}) = R_{nl}(r) Y_{lm}(\theta, \varphi), \tag{3.1}$$

where  $Y_{lm}(\theta, \varphi)$  are the spherical harmonics, the radial functions  $R_{nl}(r)$  are given in terms the Laguerre polynomials [17], [51], [57], [64]

$$R(r) = R_{nl}(r) = \frac{2}{n^2} \left( \frac{Z}{a_0} \right)^{3/2} \sqrt{\frac{(n-l-1)!}{(n+l)!}} e^{-\eta/2} \eta^l L_{n-l-1}^{2l+1}(\eta) \tag{3.2}$$

with

$$\eta = \frac{2Z}{n} \left( \frac{r}{a_0} \right), \quad a_0 = \frac{\hbar^2}{me^2} \tag{3.3}$$

and the normalization is

$$\int_0^\infty R_{nl}^2(r) r^2 dr = 1. \tag{3.4}$$

Here  $n = 1, 2, 3, \dots$  is the principal quantum number of the hydrogen-like atom in the nonrelativistic Schrödinger theory;  $l = 0, 1, \dots, n-1$  and  $m = -l, -l+1, \dots, l-1, l$  are the quantum numbers of



the angular momentum and its projection on the  $z$ -axis, respectively. The corresponding discrete energy levels in the cgs units are given by Bohr's formula

$$E = E_n = -\frac{mZ^2e^4}{2\hbar^2n^2}, \quad (3.5)$$

where  $n = 1, 2, 3, \dots$  is the principal quantum number; they do not depend on the quantum number of the orbital angular momenta  $l$  due to a “hidden”  $SO(4)$ –symmetry of the Hamiltonian of the nonrelativistic hydrogen atom; see, for example, [34], [51] and references therein and the original paper by Fock [41] and Bargmann [11].

**3.2. Matrix Elements.** In this section we evaluate the mean values

$$\langle r^p \rangle = \frac{\int_{\mathbf{R}^3} |\psi_{nlm}(\mathbf{r})|^2 r^p dv}{\int_{\mathbf{R}^3} |\psi_{nlm}(\mathbf{r})|^2 dv} = \frac{\int_0^\infty R_{nl}^2(r) r^{p+2} dr}{\int_0^\infty R_{nl}^2(r) r^2 dr}, \quad dv = r^2 dr d\omega \quad (3.6)$$

in terms of the Chebyshev polynomials of a discrete variable  $t_k(x, N) = h_k^{(0,0)}(x, N)$  [75], [76] and [77]. Here we have used the orthogonality relation for the spherical harmonics [57], [80],

$$\int_{S^2} Y_{lm}^*(\theta, \varphi) Y_{l'm'}(\theta, \varphi) d\omega = \delta_{ll'} \delta_{mm'} \quad (3.7)$$

with  $d\omega = \sin \theta d\theta d\varphi$  and  $0 \leq \theta \leq \pi, 0 \leq \varphi \leq 2\pi$ . The end results are

$$\langle r^{k-1} \rangle = \frac{1}{2n} \left( \frac{na_0}{2Z} \right)^{k-1} t_k(n-l-1, -2l-1), \quad (3.8)$$

when  $k = 0, 1, 2, \dots$  and

$$\left\langle \frac{1}{r^{k+2}} \right\rangle = \frac{1}{2n} \left( \frac{2Z}{na_0} \right)^{k+2} t_k(n-l-1, -2l-1), \quad (3.9)$$

when  $k = 0, 1, \dots, 2l$ .

Although a connection of the mean values (3.6) with a family of the hypergeometric polynomials was established by Pasternack [58], the relation with the Chebyshev polynomials of a discrete variable was missing. This is a curious but fruitful case of a “mistaken identity” in the theory of classical orthogonal polynomials. The so-called Hahn polynomials of a discrete variable were originally introduced by Chebyshev [77], they have a discrete measure on the finite equidistant set of points. Bateman, in a series of papers [12], [13], [14], [15], and Hardy [44] were the first who studied a continuous measure on the entire real line for the simplest special case of these polynomials of Chebyshev. Pasternack gave an extension of the results of Bateman to a one parameter family of the continuous orthogonal polynomials [59]. After investigation of these Bateman–Pasternack polynomials in the fifties by several authors; see [79], [86], [23], [25] and [26]; Askey and Wilson [6] introduced what nowadays known as the symmetric continuous Hahn polynomials, they have two free parameters — but one parameter had been yet missing! Finally, Suslov [67], Atakishiyev and Suslov [8] and Askey [5] have introduced the continuous Hahn polynomials in their full generality in the mid of eighties. More details on the discovery the continuous Hahn polynomials and their properties are given in [49] among other things.

Indeed, in view of the normalization condition of the Coulomb wave functions (3.4) one gets

$$\begin{aligned}\langle r^p \rangle &= \int_0^\infty R_{nl}^2(r) r^{p+2} dr \\ &= \frac{4}{n^4} \left( \frac{na_0}{2Z} \right)^{p+3} \left( \frac{Z}{a_0} \right)^3 \frac{(n-l-1)!}{(n+l)!} \int_0^\infty e^{-\eta} \eta^{p+2l+2} (L_{n-l-1}^{2l+1}(\eta))^2 d\eta\end{aligned}\quad (3.10)$$

and the last integral can be evaluated with the help of (2.10) or (2.11) giving rise to (3.8) and (3.9), respectively.

A convenient “inversion” relation for the Coulomb matrix elements,

$$\left\langle \frac{1}{r^{k+2}} \right\rangle = \left( \frac{2Z}{na_0} \right)^{2k+1} \frac{(2l-k)!}{(2l+k+1)!} \langle r^{k-1} \rangle \quad (3.11)$$

with  $0 \leq k \leq 2l$ , follows directly from (3.8) and (3.9). This relation is contained in an implicit form in [51], it was given explicitly in [58].

**3.3. Special Cases.** The explicit expression (3.8) for the matrix elements  $\langle r^p \rangle$  and the familiar three term recurrence relation for the Hahn polynomials  $h_k^{(\alpha, \beta)}(x, N)$  [55], [57],

$$x h_k^{(\alpha, \beta)}(x, N) = \alpha_k h_{k+1}^{(\alpha, \beta)}(x, N) + \beta_k h_k^{(\alpha, \beta)}(x, N) + \gamma_k h_{k-1}^{(\alpha, \beta)}(x, N) \quad (3.12)$$

with

$$\begin{aligned}\alpha_k &= \frac{(n+1)(\alpha + \beta + n + 1)}{(\alpha + \beta + 2n + 1)(\alpha + \beta + 2n + 2)}, \\ \beta_k &= \frac{\alpha - \beta + 2N - 2}{4} + \frac{(\beta^2 - \alpha^2)(\alpha + \beta + 2N)}{4(\alpha + \beta + 2n)(\alpha + \beta + 2n + 2)}, \\ \gamma_k &= \frac{(\alpha + n)(\beta + n)(\alpha + \beta + N + n)(N - n)}{(\alpha + \beta + 2n)(\alpha + \beta + 2n + 1)},\end{aligned}$$

imply the following three term recurrence relation for the matrix elements (3.6):

$$\begin{aligned}\langle r^k \rangle &= \frac{2n(2k+1)}{k+1} \left( \frac{na_0}{2Z} \right) \langle r^{k-1} \rangle \\ &\quad - \frac{k((2l+1)^2 - k^2)}{k+1} \left( \frac{na_0}{2Z} \right)^2 \langle r^{k-2} \rangle\end{aligned}\quad (3.13)$$

with the “initial conditions”

$$\left\langle \frac{1}{r} \right\rangle = \frac{Z}{a_0 n^2}, \quad \langle 1 \rangle = 1 \quad (3.14)$$

which is convenient for evaluation of the mean values  $\langle r^k \rangle$  for  $k \geq 1$  [58]. The inversion relation (3.11) can be used then for all possible negative values of  $k$ . One can easily find the following matrix elements

$$\langle r \rangle = \frac{a_0}{2Z} (3n^2 - l(l+1)), \quad (3.15)$$

$$\langle r^2 \rangle = 2 \left( \frac{na_0}{2Z} \right)^2 (5n^2 + 1 - 3l(l+1)), \quad (3.16)$$

$$\left\langle \frac{1}{r} \right\rangle = \frac{Z}{a_0 n^2}, \quad (3.17)$$

$$\left\langle \frac{1}{r^2} \right\rangle = \frac{2Z^2}{a_0^2 n^3 (2l+1)}, \quad (3.18)$$

$$\left\langle \frac{1}{r^3} \right\rangle = \frac{Z^3}{a_0^3 n^3 (l+1)(l+1/2)l}, \quad (3.19)$$

$$\left\langle \frac{1}{r^4} \right\rangle = \frac{Z^4 (3n^2 - l(l+1))}{2a_0^4 n^5 (l+3/2)(l+1)(l+1/2)l(l-1/2)}, \quad (3.20)$$

which are important in many calculations in quantum mechanics and quantum electrodynamics [1], [17], [16], [47], [82]; see [17] for more examples.

Equations (3.5) and (3.17) show that the total energy of the electron in the hydrogen-like atom is equal to half the average potential energy:

$$\langle U \rangle = -Ze^2 \left\langle \frac{1}{r} \right\rangle = -\frac{Z^2 e^2}{a_0 n^2} = 2E. \quad (3.21)$$

This is the statement of so-called virial theorem in nonrelativistic quantum mechanics; see, for example, [17], p. 165 and [51].

The average distance between the electron and the nucleus  $\bar{r} = \langle r \rangle$  is given by (3.15). The mean square deviation of the nucleus-electron separation is

$$\overline{(r - \bar{r})^2} = \overline{r^2} - \bar{r}^2 = \left( \frac{a_0}{2Z} \right)^2 (n^2(n^2 + 2) - l^2(l+1)^2). \quad (3.22)$$

The quantum mechanical analogue to Bohr orbits of large eccentricity corresponds to large values of this number (small  $l$ ).

**3.4. Screening.** Let us evaluate the effective electrostatic potential  $V(\mathbf{r})$  created by motion of the electron in a hydrogen-like atom with the nucleus of charge  $Ze$ . This result is well known in the nonrelativistic Schrödinger theory — see, for example, [45] and [57] — but we emphasize the connection with the Hahn polynomials in order to obtain similar results in the relativistic Dirac theory in the next section. For the electron in the stationary state with the wave function (3.1) and the quantum numbers  $n, l$  and  $m$  this potential is

$$V(\mathbf{r}) = \frac{Ze}{r} - e \int_{\mathbf{R}^3} \frac{|\psi_{nlm}(\mathbf{r}')|^2}{|\mathbf{r} - \mathbf{r}'|} (r')^2 dr' d\omega', \quad (3.23)$$

where  $e\rho(\mathbf{r}) = e|\psi_{nlm}(\mathbf{r})|^2$  is the average charge distribution of the electron in the atom. In order to evaluate the integral one can use the generating relation (8.15) in the form

$$\frac{1}{|\mathbf{r} - \mathbf{r}'|} = \sum_{s=0}^{\infty} \frac{r_{<}^s}{r_{>}^{s+1}} \left( \frac{4\pi}{2s+1} \sum_{m'=-s}^s Y_{sm'}^*(\theta', \varphi') Y_{sm'}(\theta, \varphi) \right), \quad (3.24)$$

where  $r_{<} = \min(r, r')$  and  $r_{>} = \max(r, r')$ ; see [57], [63], [80] for the proof of this expansion formula. In view of (3.1) one gets

$$\int_{\mathbf{R}^3} \frac{|\psi_{nlm}(\mathbf{r}')|^2}{|\mathbf{r} - \mathbf{r}'|} (r')^2 dr' d\omega' = \sum_{s=0}^{\infty} \frac{4\pi}{2s+1} \int_0^{\infty} \frac{r_{<}^s}{r_{>}^{s+1}} R_{nl}^2(r') (r')^2 dr' \quad (3.25)$$

$$\times \sum_{m'=-s}^s Y_{sm'}(\theta, \varphi) \int_{S^2} Y_{sm'}^*(\theta', \varphi') Y_{lm}^*(\theta', \varphi') Y_{lm}(\theta', \varphi') d\omega'.$$

The  $\varphi'$  integration reduces the sum over  $m'$  to a single term with  $m' = 0$  and we arrive at

$$\begin{aligned} V(\mathbf{r}) &= \frac{Ze}{r} - e \sum_{s=0}^{\infty} \frac{4\pi}{2s+1} \int_0^{\infty} \frac{r_{<}^s}{r_{>}^{s+1}} R_{nl}^2(r') (r')^2 dr' \\ &\times Y_{s0}(\theta, 0) \int_{S^2} Y_{s0}^*(\theta', \varphi') Y_{lm}^*(\theta', \varphi') Y_{lm}(\theta', \varphi') d\omega'. \end{aligned} \quad (3.26)$$

The integral of the product of three spherical harmonics can be evaluated in terms of the Clebsch–Gordan coefficients  $C_{l_1 m_1 l_2 m_2}^{lm}$  of the quantum theory of angular momentum [35], [55], [55], [63], [80], [81], [84] with the help of the product formula (8.16) and the orthogonality property (3.7). The result is

$$\int_{S^2} Y_{s0}^*(\theta', \varphi') Y_{lm}^*(\theta', \varphi') Y_{lm}(\theta', \varphi') d\omega' = \sqrt{\frac{2s+1}{4\pi}} C_{lms0}^{lm} C_{l0s0}^{l0}. \quad (3.27)$$

In view of the symmetry property of the Clebsch–Gordan coefficients [55], [63], [80]

$$C_{l_1 m_1 l_2 m_2}^{lm} = (-1)^{l_1+l_2-l} C_{l_1, -m_1, l_2, -m_2}^{l, -m} \quad (3.28)$$

and the selection rule  $|l_1 - l_2| \leq l \leq l_1 + l_2$  of the addition of two angular momenta in quantum mechanics, the integral (3.27) is not zero only for  $s = 0, 2, \dots, 2l$ . As a result

$$\begin{aligned} V(\mathbf{r}) &= \frac{Ze}{r} - e \sum_{s=0}^l \sqrt{\frac{4\pi}{4s+1}} C_{lms, 2s, 0}^{lm} C_{l0, 2s, 0}^{l0} Y_{2s, 0}(\theta, \varphi) \\ &\times \int_0^{\infty} \frac{r_{<}^{2s}}{r_{>}^{2s+1}} R_{nl}^2(r') (r')^2 dr'. \end{aligned} \quad (3.29)$$

It is known that the Clebsch–Gordan coefficients are simply the Hahn polynomials up to a normalization factor; see [55] and references therein for more details on the relation between the Clebsch–Gordan coefficients and the Hahn polynomials, which was overlooked on the early stage of developing of the quantum theory of angular momentum [27], [35], [63], [80], [81], [83], [84] and had been established much later independently by Koornwinder [50] and Smorodinskii and Suslov [65]. It is worth noting that before that Wilson [85] found that the next “building blocks” of the quantum theory of angular momentum, the so-called  $6j$ -symbols, are orthogonal polynomials of a discrete variable, see also [66], [68] and [69]; Askey and Wilson [7] studied this new orthogonal polynomials and their  $q$ -extensions in details; see also [2], [3], [42], [48], [55] and references therein for the current status of the theory of Askey–Wilson polynomials and their special and/or limiting cases. Thus the Hahn polynomials appear in the expression (3.29) for the effective electrostatic potential  $V(\mathbf{r})$  in the nonrelativistic hydrogen-like atom.

The special Clebsch–Gordan coefficients  $C_{l0, 2s, 0}^{l0}$  in (3.29) are [80]

$$C_{l0, 2s, 0}^{l0} = (-1)^s \frac{(l+s)!(2s)!}{(l-s)!(s!)^2} \sqrt{\frac{(2l+1)(2l-2s)!}{(2l+2s+1)!}} \quad (3.30)$$

and

$$Y_{2s,0}(\theta, \varphi) = \sqrt{\frac{4s+1}{4\pi}} P_{2s}(\cos \theta), \quad (3.31)$$

where  $P_n(x)$  are the Legendre polynomials.

The integral over the radial functions in (3.29) can be rewritten in the form

$$\begin{aligned} & \int_0^\infty \frac{r_{<}^{2s}}{r_{>}^{2s+1}} R_{nl}^2(r') (r')^2 dr' \\ &= \frac{1}{r^{2s+1}} \int_0^r (r')^{2s+2} R_{nl}^2(r') dr' + r^{2s} \int_r^\infty (r')^{1-2s} R_{nl}^2(r') dr' \\ &= \frac{1}{r^{2s+1}} \left( \int_0^\infty (r')^{2s+2} R_{nl}^2(r') dr' - \int_r^\infty (r')^{2s+2} R_{nl}^2(r') dr' \right) \\ &\quad + r^{2s} \int_r^\infty (r')^{1-2s} R_{nl}^2(r') dr' \\ &= \frac{1}{r^{2s+1}} J_{2s} - \frac{1}{r^{2s+1}} J_{2s}(r) + r^{2s} J_{-2s-1}(r), \end{aligned} \quad (3.32)$$

where the first integral  $J_{2s} = \langle r^{2s} \rangle$  is given by (3.8) in terms of the Chebyshev polynomials of a discrete variable. The other two integral are of the form

$$J_k(r) = \int_r^\infty (r')^{k+2} R_{nl}^2(r') dr'. \quad (3.33)$$

They are special cases of our integral (2.26) and can be evaluated by (2.29) in terms of the incomplete gamma function; they have simple asymptotics at infinity. The reader can work out the details.

For the electron in the ground state  $n = 1$  and  $l = m = 0$  all the integral are easily evaluated and the result is

$$V(r) = \frac{(Z-1)e}{r} + \left( \frac{e}{r} + \frac{Ze}{a_0} \right) e^{-2Zr/a_0}. \quad (3.34)$$

For small distances  $r \rightarrow 0$  the effective potential  $V(r) \rightarrow eZ/r$  as expected and as  $r \rightarrow \infty$  the potential  $V(r) \rightarrow e(Z-1)/r$  which is the potential of the nucleus of charge  $Ze$  screened by the electron.

#### 4. RELATIVISTIC COULOMB PROBLEM

**4.1. Dirac Equation.** The relativistic wave equation of Dirac [31], [32], [33], [38], [39]

$$i\hbar \frac{\partial}{\partial t} \psi = H\psi \quad (4.1)$$

for the electron in an external central field with the potential energy  $U(r)$  has the Hamiltonian of the form

$$H = c\boldsymbol{\alpha}\mathbf{p} + mc^2\beta + U(r), \quad (4.2)$$

where  $\boldsymbol{\alpha}\mathbf{p} = \alpha_1 p_1 + \alpha_2 p_2 + \alpha_3 p_3$  with the momentum operator  $\mathbf{p} = -i\hbar\nabla$  and

$$\boldsymbol{\alpha} = \begin{pmatrix} \mathbf{0} & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & \mathbf{0} \end{pmatrix}, \quad \beta = \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & -\mathbf{1} \end{pmatrix}, \quad \psi = \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix}. \quad (4.3)$$

We use the standard representation of the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (4.4)$$

and

$$\mathbf{0} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}, \quad \mathbf{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

The relativistic electron has a four component wave function

$$\psi = \psi(\mathbf{r}, t) = \begin{pmatrix} \mathbf{u}(\mathbf{r}, t) \\ \mathbf{v}(\mathbf{r}, t) \end{pmatrix} = \begin{pmatrix} \psi_1(\mathbf{r}, t) \\ \psi_2(\mathbf{r}, t) \\ \psi_3(\mathbf{r}, t) \\ \psi_4(\mathbf{r}, t) \end{pmatrix} \quad (4.5)$$

and the Dirac equation (4.1) is a matrix equation that is equivalent to a system of four first order partial differential equations. The inner product for two Dirac (bispinor) wave functions

$$\psi = \begin{pmatrix} \mathbf{u}_1 \\ \mathbf{v}_1 \end{pmatrix} = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix}, \quad \phi = \begin{pmatrix} \mathbf{u}_2 \\ \mathbf{v}_2 \end{pmatrix} = \begin{pmatrix} \phi_1 \\ \phi_2 \\ \phi_3 \\ \phi_4 \end{pmatrix}$$

is defined as a scalar quantity

$$\begin{aligned} \langle \psi, \phi \rangle &= \int_{\mathbf{R}^3} \psi^\dagger \phi \, dv = \int_{\mathbf{R}^3} (\mathbf{u}_1^\dagger \mathbf{u}_2 + \mathbf{v}_1^\dagger \mathbf{v}_2) \, dv \\ &= \int_{\mathbf{R}^3} (\psi_1^* \phi_1 + \psi_2^* \phi_2 + \psi_3^* \phi_3 + \psi_4^* \phi_4) \, dv \end{aligned} \quad (4.6)$$

with the squared norm

$$\begin{aligned} \|\psi\|^2 &= \langle \psi, \psi \rangle = \int_{\mathbf{R}^3} \psi^\dagger \psi \, dv = \int_{\mathbf{R}^3} (\mathbf{u}_1^\dagger \mathbf{u}_1 + \mathbf{v}_1^\dagger \mathbf{v}_1) \, dv \\ &= \int_{\mathbf{R}^3} (|\psi_1|^2 + |\psi_2|^2 + |\psi_3|^2 + |\psi_4|^2) \, dv \end{aligned} \quad (4.7)$$

and the wave functions are usually normalized so that  $\|\psi\| = \langle \psi, \psi \rangle^{1/2} = 1$ .

The substitution

$$\psi(\mathbf{r}, t) = e^{-i(E-t)/\hbar} \psi(\mathbf{r}), \quad (4.8)$$

gives the stationary Dirac equation

$$H\psi(\mathbf{r}) = E\psi(\mathbf{r}), \quad (4.9)$$

where  $E$  is the total energy of the electron.

According to Steven Weinberg ([82], vol. I, p. 565), physicists learn in kindergarten how to solve problems related to the wave equation of Dirac in the presence of external fields. In Section 6 of this paper, for the benefits of the reader who is not an expert in theoretical physics, we outline a procedure of separation of the variables and solve the corresponding first order system of radial equations for the Dirac equation in the Coulomb field  $U(r) = -Ze^2/r$ . The end results are presented in the next section; see also [1], [17], [16], [39], [47], [54], [57], [64] and references therein for more information.

**4.2. Relativistic Coulomb Wave Functions and Discrete Energy Levels.** The exact solutions of the stationary Dirac equation

$$H\psi = E\psi \quad (4.10)$$

for the Coulomb potential can be obtained in the spherical coordinates a result of a rather lengthy calculation. Remarkably the energy levels (4.16) were discovered in 1916 by Sommerfeld from the “old” Bohr quantum theory and the corresponding (bispinor) Dirac wave functions were originally found by Darwin [30] and Gordon [43] at early age of discovery of the “new” wave mechanics; see also [18] for a modern discussion of “Sommerfeld’s puzzle”. These classical results are nowadays included in all textbooks on relativistic quantum mechanics, quantum field theory and advanced texts on mathematical physics; see, for example, [1], [16], [17], [29], [47], [54] and [57]. More details are given in the last but one section of this paper. The end result is

$$\psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix} = \begin{pmatrix} \mathcal{Y}_{jm}^{\pm}(\mathbf{n}) F(r) \\ i\mathcal{Y}_{jm}^{\mp}(\mathbf{n}) G(r) \end{pmatrix}, \quad (4.11)$$

where the spinor spherical harmonics  $\mathcal{Y}_{jm}^{\pm}(\mathbf{n}) = \mathcal{Y}_{jm}^{(j \pm 1/2)}(\mathbf{n})$  are given explicitly in terms of the ordinary spherical functions  $Y_{lm}(\mathbf{n})$ ,  $\mathbf{n} = \mathbf{n}(\theta, \varphi) = \mathbf{r}/r$  and the special Clebsch–Gordan coefficients with the spin 1/2 as follows [1], [16], [63], [80]

$$\mathcal{Y}_{jm}^{\pm}(\mathbf{n}) = \begin{pmatrix} \mp \sqrt{\frac{(j+1/2) \mp (m-1/2)}{2j+(1 \pm 1)}} Y_{j \pm 1/2, m-1/2}(\mathbf{n}) \\ \sqrt{\frac{(j+1/2) \pm (m+1/2)}{2j+(1 \pm 1)}} Y_{j \pm 1/2, m+1/2}(\mathbf{n}) \end{pmatrix} \quad (4.12)$$

with the total angular momentum  $j = 1/2, 3/2, 5/2, \dots$  and  $m = -j, -j+1, \dots, j-1, j$ ; see Section 6.1 for discussion of properties of the spinor spherical harmonics in detail.

The radial functions  $F(r)$  and  $G(r)$  can be presented as [57]

$$\begin{pmatrix} F(r) \\ G(r) \end{pmatrix} = \frac{a^2 \beta^{3/2}}{\nu} \sqrt{\frac{(\varepsilon \kappa - \nu) n!}{\mu (\kappa - \nu) \Gamma(n + 2\nu)}} \xi^{\nu-1} e^{-\xi/2} \times \begin{pmatrix} f_1 & f_2 \\ g_1 & g_2 \end{pmatrix} \begin{pmatrix} \xi L_{n-1}^{2\nu+1}(\xi) \\ L_n^{2\nu-1}(\xi) \end{pmatrix}. \quad (4.13)$$

Here  $L_k^{\alpha}(\xi)$  are the Laguerre polynomials and we use the following notations  $\kappa = \pm(j+1/2)$ ,  $\nu = \sqrt{\kappa^2 - \mu^2}$ ,  $\mu = \alpha Z = Ze^2/\hbar c$ ,  $a = \sqrt{1 - \varepsilon^2}$ ,  $\varepsilon = E/mc^2$ ,  $\beta = mc/\hbar = 2\pi/\lambda$  and

$$\xi = 2a\beta r = 2\sqrt{1 - \varepsilon^2} \frac{mc}{\hbar} r. \quad (4.14)$$

The elements of  $2 \times 2$ -transition matrix in (4.13) are given by

$$f_1 = \frac{a\mu}{\varepsilon\kappa - \nu}, \quad f_2 = \kappa - \nu, \quad g_1 = \frac{a(\kappa - \nu)}{\varepsilon\kappa - \nu}, \quad g_2 = \mu. \quad (4.15)$$

This particular form of the relativistic radial functions (4.13) is due to Nikiforov and Uvarov [57]; it is very convenient for taking the nonrelativistic limit  $c \rightarrow \infty$ , see more details in Section 6.4; we shall use this form throughout the paper instead of the traditional one given in [1], [16], [17], [28] and elsewhere; cf. equation (6.82) below.

The relativistic discrete energy levels  $\varepsilon = \varepsilon_n = E_n/E_0$  with the rest mass energy  $E_0 = mc^2$  are given by the famous Sommerfeld fine structure formula

$$E_n = \frac{mc^2}{\sqrt{1 + \mu^2/(n + \nu)^2}}, \quad \mu = \alpha Z = \frac{Ze^2}{\hbar c}, \quad \nu = \sqrt{\kappa^2 - \mu^2}. \quad (4.16)$$

Here  $n = n_r = 0, 1, 2, \dots$  is the radial quantum number and  $\kappa = \pm(j + 1/2) = \pm 1, \pm 2, \pm 3, \dots$ . In the nonrelativistic limit  $c \rightarrow \infty$  one can expand the exact Sommerfeld–Dirac formula (4.16) in ascending powers of  $\mu^2 = (\alpha Z)^2$ , the first terms in this expansion are

$$\frac{E}{mc^2} = 1 - \frac{\mu^2}{2n^2} - \frac{\mu^4}{2n^4} \left( \frac{n}{j + 1/2} - \frac{3}{4} \right) + O(\mu^6), \quad \mu \rightarrow 0. \quad (4.17)$$

Here  $n = n_r + j + 1/2$  is the principal quantum number of the nonrelativistic hydrogen-like atom. The first term in this expansion is simply the rest mass energy  $E_0 = mc^2$  of the electron, the second term coincides with the energy eigenvalue in the nonrelativistic Schrödinger theory (3.5) and the third term gives the so-called fine structure of the energy levels – the correction obtained for the energy in the Pauli approximation which includes interaction of the spin of the electron with its orbital angular momentum; see [17] and [64] for further discussion of the hydrogen-like energy levels including comparison with the experimental data. One can show that in the same limit  $\mu \rightarrow 0$  the relativistic Coulomb wave functions (4.11) tend to the nonrelativistic wave functions of the Pauli theory; see, for example, [57] for more details; we shall elaborate more on this limit in Section 6.4.

We give below the explicit form of the radial wave functions (4.13) for the  $1S_{1/2}$ -state, when  $n = n_r = 0$ ,  $l = 0$ ,  $j = 1/2$  and  $\kappa = -1$ :

$$\begin{pmatrix} F(r) \\ G(r) \end{pmatrix} = \left( \frac{2Z}{a_0} \right)^{3/2} \sqrt{\frac{\nu_1 + 1}{2\Gamma(2\nu_1 + 1)}} \begin{pmatrix} -1 \\ \sqrt{\frac{1 - \nu_1}{1 + \nu_1}} \end{pmatrix} \xi_1^{\nu_1 - 1} e^{-\xi_1/2}. \quad (4.18)$$

Here  $\nu_1 = \sqrt{1 - \mu^2} = \varepsilon_1$  and  $\xi_1 = 2\sqrt{1 - \varepsilon_1^2}\beta r = 2Z(r/a_0)$ . One can see also [1], [17], [16], [30], [29], [43], [47], [54], [64] and references therein for more information on the relativistic Coulomb problem.

**4.3. Matrix Elements.** In this section we evaluate the mean values

$$\langle r^p \rangle = \frac{\int_{\mathbf{R}^3} \psi^\dagger r^p \psi \, dv}{\int_{\mathbf{R}^3} \psi^\dagger \psi \, dv} = \frac{\int_0^\infty (F^2(r) + G^2(r)) r^{p+2} \, dr}{\int_0^\infty (F^2(r) + G^2(r)) r^2 \, dr} \quad (4.19)$$

of all possible powers of  $r$  with respect to the relativistic Coulomb functions given by (4.11)–(4.13) in terms of the Hahn polynomials (8.7). First we use the orthogonality relation of the spinor spherical harmonics;

$$\int_{S^2} \left( \mathcal{Y}_{jm}^{(l)}(\mathbf{n}) \right)^\dagger \mathcal{Y}_{j'm'}^{(l')}(\mathbf{n}) \, d\omega = \delta_{jj'} \delta_{ll'} \delta_{mm'}, \quad (4.20)$$

see [1], [16], [80] or (6.6); and the explicit form of the wave functions (4.11) in order to simplify

$$\int_{\mathbf{R}^3} \psi^\dagger r^p \psi \, dv = \int_{\mathbf{R}^3} (\mathcal{Y}^\dagger(\mathbf{n}) \mathcal{Y}(\mathbf{n})) r^p (F^2(r) + G^2(r)) r^2 \, dr \, d\omega$$



$$\begin{aligned}
&= \int_{S^2} (\mathcal{Y}^\dagger(\mathbf{n}) \mathcal{Y}(\mathbf{n})) \, d\omega \int_0^\infty r^{p+2} (F^2(r) + G^2(r)) \, dr \\
&= \int_0^\infty r^{p+2} (F^2(r) + G^2(r)) \, dr.
\end{aligned} \tag{4.21}$$

More details on construction of the spinor spherical harmonics  $\mathcal{Y}_{jm}^\pm(\mathbf{n}) = \mathcal{Y}_{jm}^{(j\pm 1/2)}(\mathbf{n})$  and study of their properties are given in Section 6.4. The radial wave functions in (4.13) are normalized as follows

$$\int_0^\infty r^2 (F^2(r) + G^2(r)) \, dr = 1. \tag{4.22}$$

Thus one needs to evaluate the integral

$$\langle r^p \rangle = \int_0^\infty r^{p+2} (F^2(r) + G^2(r)) \, dr \tag{4.23}$$

only, and our final result with the notations from the previous section can be presented in the following closed form

$$\begin{aligned}
&4\mu\nu^2 (2a\beta)^p \langle r^p \rangle \\
&= a\kappa (\varepsilon\kappa + \nu) \frac{\Gamma(2\nu + p + 3)}{\Gamma(2\nu + 2)} {}_3F_2 \left( \begin{matrix} 1 - n, p + 2, -p - 1 \\ 2\nu + 2, 1 \end{matrix} \right) \\
&- 2(p + 2)\mu (\varepsilon^2\kappa^2 - \nu^2) \frac{\Gamma(2\nu + p + 2)}{\Gamma(2\nu + 2)} {}_3F_2 \left( \begin{matrix} 1 - n, p + 3, -p \\ 2\nu + 2, 2 \end{matrix} \right) \\
&+ a\kappa (\varepsilon\kappa - \nu) \frac{\Gamma(2\nu + p + 1)}{\Gamma(2\nu)} {}_3F_2 \left( \begin{matrix} -n, p + 2, -p - 1 \\ 2\nu, 1 \end{matrix} \right),
\end{aligned} \tag{4.24}$$

where the terminating generalized hypergeometric series  ${}_3F_2(1)$  are related to the Hahn and Chebyshev polynomials of a discrete variable due to (8.7).

Substituting (4.13) into (4.23) one gets

$$\begin{aligned}
C \langle r^p \rangle &= \int_0^\infty e^{-\xi} \xi^{2\nu+p} \left( (f_1 \xi L_{n-1}^{2\nu+1}(\xi) + f_2 L_n^{2\nu-1}(\xi))^2 \right. \\
&\quad \left. + (g_1 \xi L_{n-1}^{2\nu+1}(\xi) + g_2 L_n^{2\nu-1}(\xi))^2 \right) d\xi \\
&= (f_1^2 + g_1^2) \int_0^\infty e^{-\xi} \xi^{2\nu+p+2} (L_{n-1}^{2\nu+1}(\xi))^2 d\xi \\
&\quad + 2(f_1 f_2 + g_1 g_2) \int_0^\infty e^{-\xi} \xi^{2\nu+p+1} L_{n-1}^{2\nu+1}(\xi) L_n^{2\nu-1}(\xi) d\xi \\
&\quad + (f_2^2 + g_2^2) \int_0^\infty e^{-\xi} \xi^{2\nu+p} (L_n^{2\nu-1}(\xi))^2 d\xi,
\end{aligned} \tag{4.25}$$

where

$$C = 8\mu\nu^2 (2a\beta)^p \frac{(\kappa - \nu) \Gamma(2\nu + n)}{a(\varepsilon\kappa - \nu) n!} \tag{4.26}$$

and, in view of (4.15),

$$f_1^2 + g_1^2 = \frac{2a^2\kappa(\kappa - \nu)}{(\varepsilon\kappa - \nu)^2}, \quad f_1f_2 + g_1g_2 = \frac{2a\mu(\kappa - \nu)}{\varepsilon\kappa - \nu}, \quad f_2^2 + g_2^2 = 2\kappa(\kappa - \nu). \quad (4.27)$$

The two types of the integrals occuring in the calculation are given by our “master” formula (2.5) as follows

$$\begin{aligned} & \int_0^\infty e^{-\xi} \xi^{2\nu+p+2} (L_{n-1}^{2\nu+1}(\xi))^2 d\xi \\ &= \frac{\Gamma(2\nu+p+3)\Gamma(2\nu+n+1)}{(n-1)!\Gamma(2\nu+2)} {}_3F_2 \left( \begin{matrix} 1-n, p+2, -p-1 \\ 2\nu+2, 1 \end{matrix} \right), \end{aligned} \quad (4.28)$$

$$\begin{aligned} & \int_0^\infty e^{-\xi} \xi^{2\nu+p+1} L_{n-1}^{2\nu+1}(\xi) L_n^{2\nu-1}(\xi) d\xi \\ &= -\frac{(p+2)\Gamma(2\nu+p+2)\Gamma(2\nu+n+1)}{(n-1)!\Gamma(2\nu+2)} {}_3F_2 \left( \begin{matrix} 1-n, p+3, -p \\ 2\nu+2, 2 \end{matrix} \right) \end{aligned} \quad (4.29)$$

and

$$\begin{aligned} & \int_0^\infty e^{-\xi} \xi^{2\nu+p} (L_n^{2\nu-1}(\xi))^2 d\xi \\ &= \frac{\Gamma(2\nu+p+1)\Gamma(2\nu+n)}{n!\Gamma(2\nu)} {}_3F_2 \left( \begin{matrix} -n, p+2, -p-1 \\ 2\nu, 1 \end{matrix} \right). \end{aligned} \quad (4.30)$$

Substituting these integrals into (4.25) and using the identity

$$a^2n(2\nu+n) = \varepsilon^2\kappa^2 - \nu^2, \quad (4.31)$$

see Section 6.3 for the proof, one finally arrives at (4.24).

In view of (8.7), the relations with the Hahn and Chebyshev polynomials of a discrete variable are

$$\begin{aligned} 4\mu\nu^2 (2a\beta)^p \langle r^p \rangle &= a\kappa(\varepsilon\kappa + \nu) h_{p+1}^{(0,0)}(n-1, -1-2\nu) \\ &\quad - 2\frac{p+2}{p+1}\mu(\varepsilon^2\kappa^2 - \nu^2) h_p^{(1,1)}(n-1, -1-2\nu) \\ &\quad + a\kappa(\varepsilon\kappa - \nu) h_{p+1}^{(0,0)}(n, 1-2\nu), \quad p \geq 0 \end{aligned} \quad (4.32)$$

and

$$\begin{aligned} \frac{4\mu\nu^2}{(2a\beta)^{p+3}} \left\langle \frac{1}{r^{p+3}} \right\rangle &= a\kappa(\varepsilon\kappa + \nu) \frac{\Gamma(2\nu-p)}{\Gamma(2\nu+p+3)} h_{p+1}^{(0,0)}(n-1, -1-2\nu) \\ &\quad + 2\mu(\varepsilon^2\kappa^2 - \nu^2) \frac{\Gamma(2\nu-p-1)}{\Gamma(2\nu+p+2)} h_p^{(1,1)}(n-1, -1-2\nu) \\ &\quad + a\kappa(\varepsilon\kappa - \nu) \frac{\Gamma(2\nu-p-2)}{\Gamma(2\nu+p+1)} h_{p+1}^{(0,0)}(n, 1-2\nu), \quad p \geq 0. \end{aligned} \quad (4.33)$$

The averages of  $r^p$  for the relativistic hydrogen atom were evaluated by Davis [28] in a form which is slightly different from our equation (4.24). It does not appear to have been noticed that the

corresponding  ${}_3F_2$ -functions can be expressed in terms of Hahn polynomials. The ease of handling of these matrix elements for the discrete levels is greatly increased if use is made of the known properties of these polynomials [36], [48], [55], [57] and [75], [76], [77]. For instance, the difference-differentiation formula

$$\Delta h_m^{(\alpha, \beta)}(x, N) = (\alpha + \beta + m + 1) h_{m-1}^{(\alpha+1, \beta+1)}(x, N-1), \quad (4.34)$$

where  $\Delta f(x) = f(x+1) - f(x)$ , in the form

$$h_{p+1}^{(0,0)}(n, -2\nu) - h_{p+1}^{(0,0)}(n-1, -2\nu) = (p+2) h_p^{(1,1)}(n-1, -1-2\nu) \quad (4.35)$$

allows to rewrite formulas (4.32)–(4.34) in terms of the Chebyshev polynomials of a discrete variable  $t_m(x) = h_m^{(0,0)}(x, N)$  only. Use of the three term recurrence relation (3.12) simplifies evaluation of the special cases of these averages. Equation (8.8) gives asymptotic formulas for the matrix elements as  $|\kappa| \rightarrow \infty$ .

**4.4. Nonrelativistic Limit.** In the limit  $c \rightarrow \infty$  the relativistic Coulomb matrix elements given by (4.19) and (4.24) tend to the nonrelativistic ones (3.6). This can be easily shown with the help of the asymptotic formulas

$$\varepsilon\kappa \pm \nu = (\kappa \pm |\kappa|) - \frac{\kappa |\kappa| \pm (n_r + |\kappa|)^2}{2 |\kappa| (n_r + |\kappa|)^2} \mu^2 + O(\mu^4) \quad (4.36)$$

as  $\mu = Ze^2/\hbar c \rightarrow 0$ ; see Section 6.4 for more details.

**4.5. Special Cases.** Some important special cases of the relativistic matrix elements are

$$\langle r^2 \rangle = \frac{5n(n+2\nu) + 4\nu^2 + 1 - \varepsilon\kappa(2\varepsilon\kappa + 3)}{2(a\beta)^2} \quad (4.37)$$

$$\langle r \rangle = \frac{a_0}{2Z} (3\varepsilon n(n+2\nu) + \kappa(2\varepsilon\kappa - 1)), \quad (4.38)$$

$$\langle 1 \rangle = 1, \quad (4.39)$$

$$\left\langle \frac{1}{r} \right\rangle = \frac{\beta}{\mu\nu} (1 - \varepsilon^2) (\varepsilon\nu + \mu\sqrt{1 - \varepsilon^2}), \quad (4.40)$$

$$\left\langle \frac{1}{r^2} \right\rangle = \frac{2a^3\beta^2\kappa(2\varepsilon\kappa - 1)}{\mu\nu(4\nu^2 - 1)}, \quad (4.41)$$

$$\left\langle \frac{1}{r^3} \right\rangle = 2(a\beta)^3 \frac{3\varepsilon^2\kappa^2 - 3\varepsilon\kappa - \nu^2 + 1}{\nu(\nu^2 - 1)(4\nu^2 - 1)}. \quad (4.42)$$

Derivation of these closed forms requires more work than in the nonrelativistic case because of a more complicated structure of the general expression (4.24). Here are some calculation details.

The special case  $p = 0$  implies the normalization of the radial wave functions (4.22) and (4.39). Indeed,

$$\begin{aligned} 4\mu\nu^2 \langle 1 \rangle &= -4\mu(\varepsilon^2\kappa^2 - \nu^2) + a\kappa(\varepsilon\kappa + \nu)(2\nu + 2) {}_3F_2 \left( \begin{matrix} 1-n, 2, -1 \\ 2\nu+2, 1 \end{matrix} \right) \\ &\quad + a\kappa(\varepsilon\kappa - \nu) 2\nu {}_3F_2 \left( \begin{matrix} -n, 2, -1 \\ 2\nu, 1 \end{matrix} \right) \end{aligned} \quad (4.43)$$

$$\begin{aligned}
&= -4\mu (\varepsilon^2 \kappa^2 - \nu^2) + 2a\kappa (\varepsilon\kappa + \nu) (\nu + n) + 2a\kappa (\varepsilon\kappa - \nu) (\nu + n) \\
&= 4\varepsilon\kappa^2 a (\nu + n) - 4\mu (\varepsilon^2 \kappa^2 - \nu^2) = 4\mu\nu^2,
\end{aligned}$$

in view of the quantization rule

$$\varepsilon\mu = a (\nu + n), \quad (4.44)$$

which leads to the Sommerfeld–Dirac formula for the discrete energy levels (4.16); see Section 6.3 for more details on (4.44).

The special case  $p = -1$  of (4.24) reads

$$\begin{aligned}
\frac{2\mu\nu^2}{a\beta} \left\langle \frac{1}{r} \right\rangle &= a\kappa (\varepsilon\kappa + \nu) + a\kappa (\varepsilon\kappa - \nu) \\
&\quad - 2\mu (\varepsilon^2 \kappa^2 - \nu^2) \frac{\Gamma(2\nu + 1)}{\Gamma(2\nu + 2)} {}_2F_1 \left( \begin{matrix} 1 - n, 1 \\ 2\nu + 2 \end{matrix}; 1 \right),
\end{aligned} \quad (4.45)$$

where by the summation formula of Gauss (8.10)

$${}_2F_1 \left( \begin{matrix} 1 - n, 1 \\ 2\nu + 2 \end{matrix}; 1 \right) = \frac{\Gamma(2\nu + 2) \Gamma(2\nu + n)}{\Gamma(2\nu + 1) \Gamma(2\nu + n + 1)}. \quad (4.46)$$

Thus, in view of (4.31)

$$\frac{2\mu\nu^2}{a\beta} \left\langle \frac{1}{r} \right\rangle = 2a\varepsilon\kappa^2 - 2\mu a^2 n, \quad (4.47)$$

and the final use of the quantization rule (4.44) results in (4.41). Our calculation of  $\langle r^{-1} \rangle$  shows that there is no simple form of the virial theorem in the Dirac theory of relativistic electron moving in the central field of the Coulomb potential.

In the case  $p = -2$  we get

$$\frac{\mu\nu^2}{(a\beta)^2} \left\langle \frac{1}{r^2} \right\rangle = \frac{a\kappa (\varepsilon\kappa + \nu)}{2\nu + 1} + \frac{a\kappa (\varepsilon\kappa - \nu)}{2\nu - 1}, \quad (4.48)$$

which leads to (4.41).

In a similar fashion, for  $p = -3$ :

$$\begin{aligned}
\frac{4\mu\nu^2}{(2a\beta)^3} \left\langle \frac{1}{r^3} \right\rangle &= 2\mu (\varepsilon^2 \kappa^2 - \nu^2) \frac{\Gamma(2\nu - 1)}{\Gamma(2\nu + 2)} \\
&\quad + a\kappa (\varepsilon\kappa + \nu) \frac{\Gamma(2\nu)}{\Gamma(2\nu + 2)} {}_3F_2 \left( \begin{matrix} 1 - n, 2, -1 \\ 2\nu + 2, 1 \end{matrix} \right) \\
&\quad + a\kappa (\varepsilon\kappa - \nu) \frac{\Gamma(2\nu - 2)}{\Gamma(2\nu)} {}_3F_2 \left( \begin{matrix} -n, 2, -1 \\ 2\nu, 1 \end{matrix} \right) \\
&= \frac{a\kappa (\varepsilon\kappa + \nu) (2\nu + 2n)}{(2\nu + 2) (2\nu + 1) 2\nu} + \frac{a\kappa (\varepsilon\kappa - \nu) (2\nu + 2n)}{2\nu (2\nu - 1) (2\nu - 2)} + \frac{2\mu (\varepsilon^2 \kappa^2 - \nu^2)}{(2\nu + 1) 2\nu (2\nu - 1)},
\end{aligned} \quad (4.49)$$

which is simplified to (4.42).

The special case  $p = 1$  gives the average distance  $\bar{r} = \langle r \rangle$  between the electron and the nucleus in the relativistic hydrogen-like atom. One gets

$$\begin{aligned} 4\mu\nu^2 (2a\beta) \langle r \rangle &= -6\mu (\varepsilon^2 \kappa^2 - \nu^2) (2\nu + 2) {}_3F_2 \left( \begin{matrix} 1-n, 4, -1 \\ 2\nu+2, 2 \end{matrix} \right) \\ &\quad + a\kappa (\varepsilon\kappa + \nu) (2\nu + 2)_2 {}_3F_2 \left( \begin{matrix} 1-n, 3, -2 \\ 2\nu+2, 1 \end{matrix} \right) \\ &\quad + a\kappa (\varepsilon\kappa - \nu) (2\nu)_2 {}_3F_2 \left( \begin{matrix} -n, 3, -2 \\ 2\nu, 1 \end{matrix} \right), \end{aligned}$$

where

$$\begin{aligned} (2\nu + 2) {}_3F_2 \left( \begin{matrix} 1-n, 4, -1 \\ 2\nu+2, 2 \end{matrix} \right) &= 2(n + \nu), \\ (2\nu)_2 {}_3F_2 \left( \begin{matrix} -n, 3, -2 \\ 2\nu, 1 \end{matrix} \right) &= 6n^2 + 12\nu n + 4\nu^2 + 2\nu \end{aligned}$$

Thus

$$2\mu\nu^2 a\beta \langle r \rangle = a\varepsilon\kappa^2 (3n(n + 2\nu) + 2\nu^2) - a\kappa\nu^2 - 3\mu (\varepsilon^2 \kappa^2 - \nu^2) (\nu + n), \quad (4.50)$$

which can be simplified to (4.38) by a straightforward calculation with the aid of (4.31) and (4.44); we leave the details to the reader.

For  $p = 2$  :

$$\begin{aligned} 4\mu\nu^2 (2a\beta)^2 \langle r^2 \rangle &= -8\mu (\varepsilon^2 \kappa^2 - \nu^2) \frac{\Gamma(2\nu + 4)}{\Gamma(2\nu + 2)} {}_3F_2 \left( \begin{matrix} 1-n, 5, -2 \\ 2\nu+2, 2 \end{matrix} \right) \\ &\quad + a\kappa (\varepsilon\kappa + \nu) \frac{\Gamma(2\nu + 5)}{\Gamma(2\nu + 2)} {}_3F_2 \left( \begin{matrix} 1-n, 4, -3 \\ 2\nu+2, 1 \end{matrix} \right) \\ &\quad + a\kappa (\varepsilon\kappa - \nu) \frac{\Gamma(2\nu + 3)}{\Gamma(2\nu)} {}_3F_2 \left( \begin{matrix} -n, 4, -3 \\ 2\nu, 1 \end{matrix} \right), \end{aligned} \quad (4.51)$$

where

$$(2\nu + 2)_2 {}_3F_2 \left( \begin{matrix} 1-n, 5, -2 \\ 2\nu+2, 2 \end{matrix} \right) = 5n^2 + 10n\nu + 4\nu^2 + 1$$

and

$$(2\nu)_3 {}_3F_2 \left( \begin{matrix} -n, 4, -3 \\ 2\nu, 1 \end{matrix} \right) = 4(n + \nu) (5n^2 + 10n\nu + 2\nu^2 + 3\nu + 1).$$

This can be transformed to (4.37) with the help of (4.44).

**4.6. Screening.** Let us evaluate the effective electrostatic potential  $V(\mathbf{r})$  for the relativistic hydrogen-like atom. For the electron in the stationary state with the wave functions (4.11) corresponding to the total angular momentum  $j$ , its projection  $m$  and the radial quantum number  $n = n_r$  this potential is

$$V(\mathbf{r}) = \frac{Ze}{r} - e \int_{\mathbf{R}^3} \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} dv', \quad (4.52)$$

where

$$\begin{aligned} e\rho(\mathbf{r}) &= e\psi^\dagger(\mathbf{r})\psi(\mathbf{r}) = eQ_{jm}(\mathbf{n}) (F^2(r) + G^2(r)), \\ Q_{jm}(\mathbf{n}) &= (\mathcal{Y}_{jm}^\pm(\mathbf{n}))^\dagger \mathcal{Y}_{jm}^\pm(\mathbf{n}) \end{aligned} \quad (4.53)$$

is the charge distribution of the electron in the atom. We evaluate the integral with the help of the generating relation (3.24). Indeed,

$$\begin{aligned} \int_{\mathbf{R}^3} \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} (r')^2 dr' d\omega' &= \sum_{s=0}^{\infty} \frac{4\pi}{2s+1} \int_0^{\infty} \frac{r_{<}^s}{r_{>}^{s+1}} (F^2(r') + G^2(r')) (r')^2 dr' \\ &\quad \times \sum_{m'=-s}^s Y_{sm'}(\mathbf{n}) \int_{S^2} Y_{sm'}^*(\mathbf{n}') Q_{jm}(\mathbf{n}') d\omega'. \end{aligned} \quad (4.54)$$

In view of (6.17) and (3.31),

$$Q_{jm}(\theta') = \sum_{p=0}^{j-1/2} \sqrt{\frac{4\pi}{4p+1}} a_p(j, m) Y_{2p,0}(\mathbf{n}'), \quad (4.55)$$

and with the help of the orthogonality property (3.7) one gets

$$\int_{S^2} Y_{sm'}^*(\mathbf{n}') Q_{jm}(\mathbf{n}') d\omega' = \delta_{m'0} \sum_{p=0}^{j-1/2} \sqrt{\frac{4\pi}{4p+1}} a_p(j, m) \delta_{s,2p}.$$

Substitution to (4.54) gives

$$\begin{aligned} V(\mathbf{r}) &= \frac{Ze}{r} - e \sum_{s=0}^{j-1/2} P_{2s}(\cos \theta) C_{jm,2s0}^{jm} \\ &\quad \times (-1)^s \sqrt{\frac{(2j+2s+1)(2j-2s)!}{(2j+1)(2j+2s)!}} \frac{(j+s-1/2)!(2s)!}{(j-s-1/2)!(s!)^2} \\ &\quad \times \int_0^{\infty} \frac{r_{<}^{2s}}{r_{>}^{2s+1}} (F^2(r') + G^2(r')) (r')^2 dr'. \end{aligned} \quad (4.56)$$

with the help of (6.18).

The integral over the radial functions in (4.56) can be rewritten in the form

$$\int_0^{\infty} \frac{r_{<}^{2s}}{r_{>}^{2s+1}} (F^2(r') + G^2(r')) (r')^2 dr' \quad (4.57)$$

$$\begin{aligned}
&= \frac{1}{r^{2s+1}} \int_0^r (r')^{2s+2} (F^2(r') + G^2(r')) dr' \\
&\quad + r^{2s} \int_r^\infty (r')^{1-2s} (F^2(r') + G^2(r')) dr' \\
&= \frac{1}{r^{2s+1}} \int_0^\infty (r')^{2s+2} (F^2(r') + G^2(r')) dr' \\
&\quad - \frac{1}{r^{2s+1}} \int_r^\infty (r')^{2s+2} (F^2(r') + G^2(r')) dr' \\
&\quad + r^{2s} \int_r^\infty (r')^{1-2s} (F^2(r') + G^2(r')) dr',
\end{aligned}$$

where the first integral is given by (4.24). The next two can be evaluated with the help of (2.29).

For the electron in the  $1S_{1/2}$ -state with the radial functions (4.18) the result is

$$\begin{aligned}
V(r) &= \frac{(Z-1)e}{r} + \frac{e(2Z/a_0)^{2\nu_1}}{\Gamma(2\nu_1+1)} r^{2\nu_1-1} e^{-2Zr/a_0} \\
&\quad + \frac{\Gamma(2\nu_1, 2Zr/a_0)}{\Gamma(2\nu_1+1)} \left( \frac{2\nu_1 e}{r} - \frac{2Ze}{a_0} \right),
\end{aligned} \tag{4.58}$$

where  $\nu_1 = \sqrt{1 - \mu^2}$ . For small distances  $r \rightarrow 0$  the effective potential  $V(r) \rightarrow eZ/r$  and as  $r \rightarrow \infty$  the potential  $V(r) \rightarrow e(Z-1)/r$  which is the potential of the nucleus of charge  $Ze$  screened by the electron. In the limit  $c \rightarrow \infty$  one gets the nonrelativistic formula (3.34).

## 5. SPECIAL FUNCTIONS AND QUANTUM MECHANICS

In this section we give a short summary of Nikiforov and Uvarov's approach to special functions of mathematical physics and their applications in quantum mechanics [57].

**5.1. Generalized Equation of Hypergeometric Type.** The second order differential equation of the form

$$u'' + \frac{\tilde{\tau}(z)}{\sigma(z)} u' + \frac{\tilde{\sigma}(z)}{\sigma^2(z)} u = 0, \tag{5.1}$$

where  $\sigma(z)$  and  $\tilde{\sigma}(z)$  are polynomials of degree at most 2 and  $\tilde{\tau}(z)$  is a polynomial of degree at most 1 of a complex variable  $z$ , is called the *generalized equation of hypergeometric type*. By the substitution  $u = \varphi(z)y$  equation (5.1) can be reduced to the *equation of hypergeometric type*

$$\sigma(z)y'' + \tau(z)y' + \lambda y = 0, \tag{5.2}$$

where  $\tau(z)$  is a polynomial of degree at most 1, and  $\lambda$  is a constant. The factor  $\varphi(z)$  here satisfies

$$\frac{\varphi'}{\varphi} = \frac{\pi(z)}{\sigma(z)}, \tag{5.3}$$

where  $\pi(z)$  is a polynomial of degree at most 1 given by a quadratic formula

$$\pi(z) = \frac{\sigma' - \tilde{\tau}}{2} \pm \sqrt{\left(\frac{\sigma' - \tilde{\tau}}{2}\right)^2 - \tilde{\sigma} + k\sigma} \tag{5.4}$$

and constant  $k$  is determined by the condition that the discriminant of the quadratic polynomial under the square root sign is zero. Then  $\tau(z)$  and  $\lambda$  are determined by

$$\tau(z) = \tilde{\tau}(z) + 2\pi(z), \quad \lambda = k + \pi'(z). \quad (5.5)$$

Two exceptions are [57]:

- (1) If  $\sigma(z)$  has a double root,  $\sigma(z) = (z - a)^2$ , the original equation can be carried out into a generalized equation of hypergeometric type with  $\sigma(s) = s$ , by a substitution  $s = (z - a)^{-1}$ .
- (2) If  $\sigma(z) = 1$  and  $(\tilde{\tau}(z)/2)^2 - \tilde{\sigma}(z)$  is a polynomial of degree 1, the substitution  $\pi(z) = -\tilde{\tau}(z)/2$  reduces the original equation to the form

$$y'' + (az + b)y = 0. \quad (5.6)$$

The linear transformation  $s = az + b$  takes this into a Lommel equation (5.68).

Solutions of (5.1)–(5.2) are known as special functions of hypergeometric type; they include classical orthogonal polynomials, hypergeometric and confluent hypergeometric functions, Hermite functions, Bessel functions and spherical harmonics. These functions are often called special functions of mathematical physics.

**5.2. Classical Orthogonal Polynomials.** The Jacobi, Laguerre and Hermite polynomials are the simplest solutions of the equation of hypergeometric type. By differentiating (5.2) we verify that the function  $v_1 = y'(z)$  satisfy the equation of the same type

$$\sigma(z) v_1'' + \tau_1(z) v_1' + \mu_1 v_1 = 0, \quad (5.7)$$

where  $\tau_1(z) = \tau(z) + \sigma'(z)$  is a polynomial of degree at most 1, and  $\mu_1 = \lambda + \tau'(z)$  is a constant.

The converse is also true: any solution of (5.7) is the derivative of a solution of (5.2) if  $\lambda = \mu_1 - \tau' \neq 0$ . Let  $v_1(z)$  be a solution of (5.7) and define the function

$$y(z) = -\frac{1}{\lambda} (\sigma(z) v_1' + \tau(z) v_1).$$

Then

$$\lambda y' = -(\sigma v_1'' + \tau_1 v_1' + \tau' v_1) = \lambda v_1$$

or  $v_1 = y'(z)$  and, therefore,  $y(z)$  satisfy (5.2).

By differentiating (5.2)  $n$  times we obtain an equation of hypergeometric type for the function  $v_n = y^{(n)}(z)$ ,

$$\sigma(z) v_n'' + \tau_n(z) v_n' + \mu_n v_n = 0, \quad (5.8)$$

where

$$\tau_n(z) = \tau(z) + n\sigma'(z), \quad (5.9)$$

$$\mu_n = \lambda + n\tau' + \frac{1}{2}n(n-1)\sigma''. \quad (5.10)$$

This property lets us construct the simplest solutions of (5.2) corresponding to some values of  $\lambda$ . Indeed, when  $\mu_n = 0$  equation (5.8) has the trivial solution  $v_n = \text{constant}$ . Since  $v_n(z) = y^{(n)}(z)$ , the equation (5.2) has a particular solution  $y = y_n(z)$  which is a polynomial of degree  $n$  if

$$\lambda = \lambda_n = -n\tau' - \frac{1}{2}n(n-1)\sigma'' \quad (n = 0, 1, 2, \dots). \quad (5.11)$$



To find these polynomials explicitly let us rewrite equations (5.2) and (5.8) in the self-adjoint forms

$$(\sigma \rho y')' + \lambda \rho y = 0, \quad (5.12)$$

$$(\sigma \rho_n v_n')' + \mu_n \rho_n v_n = 0. \quad (5.13)$$

Functions  $\rho(z)$  and  $\rho_n(z)$  satisfy the first order differential equations

$$(\sigma \rho)' = \tau \rho, \quad (5.14)$$

$$(\sigma \rho_n)' = \tau_n \rho_n. \quad (5.15)$$

So,

$$\frac{(\sigma \rho_n)'}{\rho_n} = \tau + n \sigma' = \frac{(\sigma \rho)'}{\rho} + n \sigma',$$

whence

$$\frac{\rho_n'}{\rho_n} = \frac{\rho'}{\rho} + n \frac{\sigma'}{\sigma}$$

and, consequently,

$$\rho_n(z) = \sigma^n(z) \rho(z). \quad (5.16)$$

Since  $\sigma \rho_n = \rho_{n+1}$  and  $v_n' = v_{n+1}$  one can rewrite (5.13) in the form

$$\rho_n v_n = -\frac{1}{\mu_n} (\rho_{n+1} v_{n+1})'.$$

Hence we obtain successively

$$\begin{aligned} \rho y &= \rho_0 v_0 = -\frac{1}{\mu_0} (\rho_1 v_1)' \\ &= \left(-\frac{1}{\mu_0}\right) \left(-\frac{1}{\mu_1}\right) (\rho_2 v_2)'' \\ &\vdots \\ &= \frac{1}{A_n} (\rho_n v_n)^{(n)}, \end{aligned}$$

where

$$A_0 = 1, \quad A_n = (-1)^n \prod_{k=0}^{n-1} \mu_k. \quad (5.17)$$

If  $y = y_n(z)$  is a polynomial of degree  $n$ , then  $v_n = y_n^{(n)}(z) = \text{constant}$  and we arrive at the *Rodrigues formula* for polynomial solutions of (5.2),

$$y_n(z) = \frac{B_n}{\rho(z)} (\sigma^n(z) \rho(z))^{(n)}, \quad (5.18)$$

where  $B_n = A_n^{-1} y_n^{(n)}$  is a constant. These solutions correspond to the eigenvalues (5.11).

The polynomial solutions of (5.2) obey an orthogonality property. Let us write equations for polynomials  $y_n(x)$  and  $y_m(x)$  in the self-adjoint form

$$(\sigma(x) \rho(x) y_n'(x))' + \lambda_n \rho(x) y_n(x) = 0,$$

$$(\sigma(x) \rho(x) y_m'(x))' + \lambda_m \rho(x) y_m(x) = 0,$$

multiply the first equation by  $y_m(x)$  and the second by  $y_n(x)$ , subtract the second equality from the first one and then integrate the result over  $x$  on the interval  $(a, b)$ . Since

$$\begin{aligned} & y_m(x) (\sigma(x) \rho(x) y_n'(x))' - y_n(x) (\sigma(x) \rho(x) y_m'(x))' \\ &= \frac{d}{dx} [\sigma(x) \rho(x) W(y_m(x), y_n(x))], \end{aligned}$$

where  $W(u, v) = uv' - vu'$  is the Wronskian, we get

$$(\lambda_m - \lambda_n) \int_a^b y_m(x) y_n(x) \rho(x) dx = [\sigma(x) \rho(x) W(y_m(x), y_n(x))]_{x=a}^b. \quad (5.19)$$

If the conditions

$$\sigma(x) \rho(x) x^k \Big|_{x=a,b} = 0, \quad k = 0, 1, 2, \dots \quad (5.20)$$

are satisfied for some points  $a$  and  $b$ , then the right hand side of (5.19) vanishes because the Wronskian is a polynomial in  $x$ . Therefore, we arrive at the *orthogonality property*

$$\int_a^b y_m(x) y_n(x) \rho(x) dx = 0 \quad (5.21)$$

provided that  $\lambda_m \neq \lambda_n$ . One can replace this condition by  $m \neq n$  due to the relation  $\lambda_m - \lambda_n = (m - n)(\tau' + (n + m - 1)\sigma''/2)$  if  $\tau' + (n + m - 1)\sigma''/2 \neq 0$ .

We shall refer to polynomial solutions of (5.2) obeying the orthogonality property (5.21) with respect to a positive weight function  $\rho(x)$  on a real interval  $(a, b)$  as *classical orthogonal polynomials*.

Equation

$$(\sigma(x) \rho(x))' = \tau(x) \rho(x) \quad (5.22)$$

for the weight function  $\rho(x)$  is usually called the *Pearson equation*. By using the linear transformations of independent variable  $x$  one can reduce solutions of (5.22) to the following canonical forms

$$\rho(x) = \begin{cases} (1-x)^\alpha (1+x)^\beta & \text{for } \sigma(x) = 1-x^2, \\ x^\alpha e^{-x} & \text{for } \sigma(x) = x, \\ e^{-x^2} & \text{for } \sigma(x) = 1. \end{cases} \quad (5.23)$$

The corresponding orthogonal polynomials are the *Jacobi polynomials*  $P_n^{(\alpha, \beta)}(x)$ , the *Laguerre polynomials*  $L_n^\alpha(x)$  and the *Hermite polynomials*  $H_n(x)$ .

The basic information about the classical orthogonal polynomials is given in Table, which contains also the leading coefficients in the expansion  $y_n(x) = a_n x^n + b_n x^{n-1} + \dots$ , the squared norms

$$d_n^2 = \int_a^b y_n^2(x) \rho(x) dx \quad (5.24)$$

and the coefficients of the three-term recurrence relation

$$x y_n(x) = \alpha_n y_{n+1}(x) + \beta_n y_n(x) + \gamma_n y_{n-1}(x) \quad (5.25)$$

with

$$\alpha_n = \frac{a_n}{a_{n+1}}, \quad \beta_n = \frac{b_n}{a_n} - \frac{b_{n+1}}{a_{n+1}}, \quad \gamma_n = \alpha_{n-1} \frac{d_n^2}{d_{n-1}^2}. \quad (5.26)$$

$y_n(x)$	$P_n^{(\alpha, \beta)}(x) (\alpha > -1, \beta > -1)$	$L_n^\alpha(x) (\alpha > -1)$	$H_n(x)$
$(a, b)$	$(-1, 1)$	$(0, \infty)$	$(-\infty, \infty)$
$\rho(x)$	$(1-x)^\alpha(1+x)^\beta$	$x^\alpha e^{-x}$	$e^{-x^2}$
$\sigma(x)$	$1-x^2$	$x$	$1$
$\tau(x)$	$\beta - \alpha - (\alpha + \beta + 2)x$	$1 + \alpha - x$	$-2x$
$\lambda_n$	$n(\alpha + \beta + n + 1)$	$n$	$2n$
$B_n$	$\frac{(-1)^n}{2^n n!}$	$\frac{1}{n!}$	$(-1)^n$
$a_n$	$\frac{\Gamma(\alpha + \beta + 2n + 1)}{2^n n! \Gamma(\alpha + \beta + n + 1)}$	$\frac{n!}{(-1)^n}$	$2^n$
$b_n$	$\frac{(\alpha - \beta) \Gamma(\alpha + \beta + 2n)}{2^n (n-1)! \Gamma(\alpha + \beta + n + 1)}$	$(-1)^{n-1} \frac{\alpha + n}{(n-1)!}$	$0$
$d^2$	$\frac{2^{\alpha+\beta+1} \Gamma(\alpha + n + 1) \Gamma(\beta + n + 1)}{n! (\alpha + \beta + 2n + 1) \Gamma(\alpha + \beta + n + 1)}$	$\frac{\Gamma(\alpha + n + 1)}{n!}$	$2^n n! \sqrt{\pi}$
$\alpha_n$	$\frac{2(n+1)(\alpha + \beta + n + 1)}{(\alpha + \beta + 2n + 1)(\alpha + \beta + 2n + 2)}$	$-(n+1)$	$\frac{1}{2}$
$\beta_n$	$\frac{\beta^2 - \alpha^2}{(\alpha + \beta + 2n)(\alpha + \beta + 2n + 2)}$	$\alpha + 2n + 1$	$0$
$\gamma_n$	$\frac{2(\alpha + n)(\beta + n)}{(\alpha + \beta + 2n)(\alpha + \beta + 2n + 1)}$	$-(\alpha + n)$	$n$

More details about the Jacobi, Laguerre and Hermite polynomials and their numerous extensions can be found in [3], [7], [42], [48], [55], [57], [71], [74] and references therein.

**5.3. Classical Orthogonal Polynomials and Eigenvalue Problems.** The following theorem is a useful tool for finding of the square integrable solutions of basic problems in quantum mechanics [57].

**Theorem 1.** *Let  $y = y(x)$  be a solution of the equation of hypergeometric type (5.2) and let  $\rho(x)$ , a solution of the Pearson equation (5.22), be bounded on the interval  $(a, b)$  and satisfy the boundary conditions (5.20). Then nontrivial solutions of (5.2) such that  $y(x) \sqrt{\rho(x)}$  is bounded and of integrable square on  $(a, b)$  exist only for the eigenvalues given by (5.11); they are the corresponding classical orthogonal polynomials on  $(a, b)$  and can be found by the Rodrigues-type formula (5.18).*

The proof is given in [57].

**5.4. Integral Representation for Special Functions.** The differential equation of hypergeometric type (5.2) can be rewritten in self-adjoint form

$$(\sigma(z) \rho(z) y'(z))' + \lambda \rho(z) y(z) = 0, \quad (5.27)$$

where  $\rho(z)$  satisfies the first order equation

$$(\sigma(z) \rho(z))' = \tau(z) \rho(z). \quad (5.28)$$

Nikiforov and Uvarov [57] suggested to construct particular solutions of the differential equation of hypergeometric type (5.2) in a form of a general integral representation for special functions of hypergeometric type as a refinement of the Laplace method. A slightly modified version of their main theorem is

**Theorem 2.** *Let  $\rho(z)$  satisfy (5.28) and  $\nu$  be a root of the equation*

$$\lambda + \nu\tau' + \frac{1}{2}\nu(\nu - 1)\sigma'' = 0. \quad (5.29)$$

*Then the differential equation (5.2) has a particular solution of the form*

$$y(z) = y_\nu(z) = \frac{C_\nu}{\rho(z)} \int_C \frac{\sigma^\nu(s) \rho(s)}{(s-z)^{\nu+1}} ds, \quad (5.30)$$

*where  $C_\nu$  is a constant and  $C$  is a contour in the complex  $s$ -plane, if:*

(1) *the derivative of the integral*

$$\varphi_{\nu\mu}(z) = \int_C \frac{\rho_\nu(s)}{(s-z)^{\mu+1}} ds \quad \text{with} \quad \rho_\nu(s) = \sigma^\nu(s) \rho(s) \quad (5.31)$$

*can be evaluated for  $\mu = \nu - 1$  and  $\mu = \nu$  by using the formula*

$$\varphi'_{\nu\mu}(z) = (\mu + 1) \varphi_{\nu, \mu+1}(z); \quad (5.32)$$

(2) *the contour  $C$  is chosen so that the equality*

$$\left. \frac{\sigma^{\nu+1}(s) \rho(s)}{(s-z)^{\nu+1}} \right|_{s_1}^{s_2} = 0 \quad (5.33)$$

*holds, where  $s_1$  and  $s_2$  are end points of the contour  $C$ .*

We present here a simple proof of this theorem [71], which is different from one in [57].

*Proof.* The function  $\rho_\nu(s) = \sigma^\nu(s) \rho(s)$  satisfy the equation

$$(\sigma(s) \rho_\nu(s))' = \tau_\nu(s) \rho_\nu(s), \quad (5.34)$$

where  $\tau_\nu(s) = \tau(s) + \nu\sigma'(s)$ . We multiply both sides of this equality by  $(s-z)^{-\nu-1}$  and integrate over contour  $C$ . Upon integrating by parts we obtain

$$\left. \frac{\sigma(s) \rho_\nu(s)}{(s-z)^{\nu+1}} \right|_{s_1}^{s_2} + (\nu+1) \int_C \frac{\sigma(s) \rho_\nu(s)}{(s-z)^{\nu+2}} ds = \int_C \frac{\tau_\nu(s) \rho_\nu(s)}{(s-z)^{\nu+1}} ds. \quad (5.35)$$

By hypothesis, the first term is equal to zero. We expand polynomials  $\sigma(s)$  and  $\tau_\nu(s)$  in powers of  $s-z$ :

$$\begin{aligned} \sigma(s) &= \sigma(z) + \sigma'(z)(s-z) + \frac{1}{2}\sigma''(z)(s-z)^2, \\ \tau_\nu(s) &= \tau_\nu(z) + \tau'_\nu(z)(s-z). \end{aligned}$$

Taking into account the integral formulas for the functions  $\varphi_{\nu, \nu-1}(z)$ ,  $\varphi_{\nu\nu}(z)$  and  $\varphi_{\nu, \nu+1}(z)$ , we arrive at the relation

$$(\nu+1) \left( \sigma(z) \varphi_{\nu, \nu+1} + \sigma'(z) \varphi_{\nu\nu} + \frac{1}{2}\sigma''(z) \varphi_{\nu, \nu-1} \right) = \tau_\nu(z) \varphi_{\nu\nu} + \tau'_\nu(z) \varphi_{\nu, \nu-1}.$$

Upon substituting  $\tau_\nu = \tau + \nu\sigma'$  and using the formula  $\varphi'_{\nu\nu} = (\nu + 1)\varphi_{\nu, \nu+1}$  one gets

$$\sigma\varphi'_{\nu\nu} + (\sigma' - \tau)\varphi_{\nu\nu} = \left(\tau' + \frac{1}{2}(\nu - 1)\sigma''\right)\varphi_{\nu, \nu-1}. \quad (5.36)$$

At the same time, by differentiating the relation  $\sigma\rho y' = C_\nu\sigma\varphi_{\nu\nu}$  we find that

$$\frac{1}{C_\nu}\sigma\rho y' = \sigma\varphi'_{\nu\nu} + (\sigma' - \tau)\varphi_{\nu\nu}. \quad (5.37)$$

Comparing (5.36) and (5.37) we obtain

$$\sigma\rho y' = \kappa_\nu C_\nu\varphi_{\nu, \nu-1}, \quad (5.38)$$

where  $\kappa_\nu = \tau' + (\nu - 1)\sigma''/2$ . Upon differentiating (5.38) we arrive to the equation of hypergeometric type in the self-adjoint form

$$(\sigma\rho y')' + \lambda\rho y = 0,$$

where  $\lambda = -\nu\kappa_\nu = -\nu\tau' - \nu(\nu - 1)\sigma''/2$ . This proves the theorem.  $\square$

In the proof of Theorem 2 we have, en route, deduced the formula (5.38), which is a simple integral representation for the first derivative of the function of hypergeometric type:

$$y'_\nu(z) = \frac{C_\nu^{(1)}}{\sigma(z)\rho(z)} \int_C \frac{\rho_\nu(s)}{(s-z)^\nu} ds, \quad (5.39)$$

where  $C_\nu^{(1)} = \kappa_\nu C_\nu = \left(\tau' + \frac{1}{2}(\nu - 1)\sigma''\right)C_\nu$ . Hence

$$y_\nu^{(k)}(z) = \frac{C_\nu^{(k)}}{\rho_k(z)} \varphi_{\nu, \nu-k}(z) = \frac{C_\nu^{(k)}}{\sigma^k(z)\rho(z)} \int_C \frac{\rho_\nu(s)}{(s-z)^{\nu-k+1}} ds, \quad (5.40)$$

where  $C_\nu^{(k)} = \prod_{p=0}^{k-1} \left(\tau' + \frac{1}{2}(\nu + p - 1)\sigma''\right)C_\nu$ .

See [56], [71] and [72] for an extension of this theorem to the case of the so-called difference equation of hypergeometric type on nonuniform lattices.

**5.5. Power Series Method.** We can construct particular solutions of equation (5.2) by using the power series method; see, for example, the classical work of Boole [21].

**Theorem 3.** *Let  $a$  be a root of the equation  $\sigma(z) = 0$ . Then Eq. (5.2) has a particular solution of the form*

$$y(z) = \sum_{n=0}^{\infty} c_n(z-a)^n, \quad (5.41)$$

where

$$\frac{c_{n+1}}{c_n} = -\frac{\lambda + n(\tau' + (n-1)\sigma''/2)}{(n+1)(\tau(a) + n\sigma'(a))}, \quad (5.42)$$

if:

$$(1) \quad \lim_{m \rightarrow \infty} \frac{d^k}{dx^k} y_m(x) = \frac{d^k}{dx^k} y(x) \text{ with } k = 0, 1, 2;$$

$$(2) \quad \lim_{m \rightarrow \infty} (\lambda - \lambda_m) c_m (x - a)^m = 0.$$

(Here  $y_m(x) = \sum_{n=0}^m c_n (x - a)^n$  and  $\lambda_m = -m\tau' - \frac{1}{2}m(m-1)\sigma''$ .)

In the case  $\sigma(z) = \text{constant} \neq 0$  series (5.41) satisfies (5.2) when  $a$  is a root of the equation  $\tau(z) = 0$ ,

$$\frac{c_{n+2}}{c_n} = -\frac{\lambda + n\tau'}{(n+1)(n+2)\sigma} \quad (5.43)$$

and convergence conditions (1)–(2) are valid.

*Proof.* The proof of the theorem relays on the identity

$$\begin{aligned} \rho^{-1} \frac{d}{dz} \left( \sigma \rho \frac{d}{dz} (z - \xi)^n \right) &= \left( \sigma(z) \frac{d^2}{dz^2} + \tau(z) \frac{d}{dz} \right) (z - \xi)^n \\ &= n(n-1)\sigma(\xi)(z - \xi)^{n-2} + n\tau_{n-1}(\xi)(z - \xi)^{n-1} - \lambda_n(z - \xi)^n, \end{aligned} \quad (5.44)$$

where  $\tau_m(\xi) = \tau(\xi) + m\sigma'(\xi)$  and  $\lambda_n = -n\tau' - n(n-1)\sigma''/2$ , which can be easily verified.

In fact, for a partial sum of the series (5.41) we can write

$$\begin{aligned} \left( \sigma(z) \frac{d^2}{dz^2} + \tau(z) \frac{d}{dz} + \lambda \right) y_m(z) &= \sigma(a) \sum_{n=0}^m c_n n(n-1)(z-a)^{n-2} \\ &\quad + \sum_{n=0}^m c_n n\tau_{n-1}(a)(z-a)^{n-1} + \sum_{n=0}^m c_n (\lambda - \lambda_n)(z-a)^n. \end{aligned} \quad (5.45)$$

By the hypothesis  $\sigma(a) = 0$  and the first term in the right hand side is equal to zero. Equating the coefficients in the next two terms with the aid of

$$\frac{c_{n+1}}{c_n} = \frac{\lambda_n - \lambda}{(n+1)\tau_n(a)}, \quad (5.46)$$

which is equivalent to (5.42), one gets

$$\left( \sigma(z) \frac{d^2}{dz^2} + \tau(z) \frac{d}{dz} + \lambda \right) y_m(z) = c_m (\lambda - \lambda_m) (z - a)^m. \quad (5.47)$$

Taking the limit  $m \rightarrow \infty$  we prove the first part of the theorem under the convergence conditions (1)–(2).

When  $\sigma = \text{constant}$  we can obtain in the same manner

$$\begin{aligned} \left( \sigma(z) \frac{d^2}{dz^2} + \tau(z) \frac{d}{dz} + \lambda \right) y_m(z) \\ &= \sigma \sum_{n=0}^m c_n n(n-1)(z-a)^{n-2} + \sum_{n=0}^m c_n (\lambda - \lambda_n)(z-a)^n \\ &= c_m (\lambda - \lambda_m) (z-a)^m, \end{aligned} \quad (5.48)$$

which proves the second part of the theorem in the limit  $m \rightarrow \infty$ . □

**Corollary.** Equation (5.2) has polynomial solutions  $y_m(x)$  corresponding to the eigenvalues  $\lambda = \lambda_m = -m\tau' - m(m-1)\sigma''/2$ ,  $m = 0, 1, 2, \dots$ .

This follows from (5.47) and (5.48).

**Examples.** With the aid of linear transformations of the independent variable, equation (5.2) for  $\tau' \neq 0$  can be reduced to one of the following *canonical forms* [57]:

$$z(1-z)y'' + [\gamma - (\alpha + \beta + 1)z]y' - \alpha\beta y = 0, \quad (5.49)$$

$$zy'' + (\gamma - z)y' - \alpha y = 0, \quad (5.50)$$

$$y'' - 2zy' + 2\nu y = 0. \quad (5.51)$$

According to (5.41)–(5.43) the appropriate particular solutions are:

the *hypergeometric function*,

$$y(z) = {}_2F_1(\alpha, \beta; \gamma; z) = \sum_{n=0}^{\infty} \frac{(\alpha)_n(\beta)_n}{(\gamma)_n n!} z^n, \quad (5.52)$$

the *confluent hypergeometric function*,

$$y(z) = {}_1F_1(\alpha; \gamma; z) = \sum_{n=0}^{\infty} \frac{(\alpha)_n}{(\gamma)_n n!} z^n, \quad (5.53)$$

and the *Hermite function*,

$$\begin{aligned} y(z) = H_\nu(z) &= \frac{1}{2\Gamma(-\nu)} \sum_{n=0}^{\infty} \Gamma\left(\frac{n-\nu}{2}\right) \frac{(-2z)^n}{n!} \\ &= \frac{2^\nu \Gamma(\frac{1}{2})}{\Gamma(\frac{1-\nu}{2})} {}_1F_1\left(-\frac{\nu}{2}; \frac{1}{2}; z^2\right) + \frac{2^\nu \Gamma(-\frac{1}{2})}{\Gamma(-\frac{\nu}{2})} z {}_1F_1\left(\frac{1-\nu}{2}; \frac{3}{2}; z^2\right), \end{aligned} \quad (5.54)$$

respectively. Here  $(a)_n = a(a+1)\dots(a+n-1) = \Gamma(a+n)/\Gamma(a)$  and  $\Gamma(a)$  is the gamma function of Euler.

Generally speaking, these solutions arise under certain restrictions on the variable and parameters; see equation (8.1) below for more details. They can be extended to wider domains by analytic continuation.

**Extended Power Series Method.** The solution (5.41)–(5.42) can be rewritten in the following explicit form

$$y(z) = c_0 \sum_{n=0}^{\infty} \prod_{k=0}^{n-1} \frac{(\lambda - \lambda_k)(a - z)}{\tau_k(a)(k+1)}, \quad (5.55)$$

where  $c_0$  is a constant. Using the expansion

$$y(z) = \sum_n c_n (z - \xi)^{\alpha+n}, \quad \frac{c_{n+1}}{c_n} = \frac{\lambda_{\alpha+n} - \lambda}{(\alpha + n + 1)\tau_{\alpha+n}(a)} \quad (5.56)$$

one can construct solutions of the more general form

$$y(z) = c_0 (z - a)^\alpha \sum_{n=0}^{\infty} \prod_{k=0}^{n-1} \frac{(\lambda - \lambda_{\alpha+k})(a - z)}{\tau_{\alpha+k}(a)(\alpha + k + 1)}, \quad (5.57)$$

provided that  $\sigma(a) = 0$  and  $\alpha \tau_{\alpha-1}(a) = 0$ . In particular, putting  $\alpha = 0$  we recover (5.55).

We can also satisfy (5.2) by using the series of the form

$$y(x) = \sum_n \frac{c_n}{(x - \xi)^{\alpha+n}}, \quad \frac{c_{n+1}}{c_n} = \frac{(\alpha + n) \tau_{-\alpha-n-1}(a)}{\lambda - \lambda_{-\alpha-n-1}}, \quad (5.58)$$

if  $\sigma(a) = 0$  and  $\lambda = \lambda_{-\alpha}$ . Hence

$$y(z) = \frac{c_0}{(z - a)^\alpha} \sum_{n=0}^{\infty} \prod_{k=0}^{n-1} \frac{(\alpha + k) \tau_{-\alpha-k-1}(a)}{(\lambda - \lambda_{-\alpha-k-1})(z - a)}. \quad (5.59)$$

When  $\sigma = \text{constant} \neq 0$  one can write the solution as

$$y(x) = \sum_n \frac{c_n}{(x - a)^{\alpha+n}}, \quad \frac{c_{n+2}}{c_n} = -\frac{(\alpha + n)(\alpha + n + 1)\sigma}{\lambda - \lambda_{-\alpha-n-2}}, \quad (5.60)$$

if  $\tau(a) = 0$  and  $\lambda = \lambda_{-\alpha}$  (for even integer values of  $n$ ) or  $\lambda = \lambda_{-\alpha-1}$  (for odd integer values of  $n$ ). This method allows to construct the fundamental set of solutions of equation (5.2). Examples are given in [73]. See [9] and [72] for an extension of the power series method to the case of the difference equation of hypergeometric type on nonuniform lattices.

**5.6. Integrals for Hypergeometric and Bessel Functions.** Using Theorem 2 one can obtain integral representations for all the most commonly used special functions of hypergeometric type, in particular, for the hypergeometric functions:

$${}_2F_1(\alpha, \beta; \gamma; z) = \frac{\Gamma(\gamma)}{\Gamma(\alpha)\Gamma(\gamma - \alpha)} \int_0^1 t^{\alpha-1} (1 - t)^{\gamma-\alpha-1} (1 - zt)^{-\beta} dt, \quad (5.61)$$

$${}_1F_1(\alpha; \gamma; z) = \frac{\Gamma(\gamma)}{\Gamma(\alpha)\Gamma(\gamma - \alpha)} \int_0^1 t^{\alpha-1} (1 - t)^{\gamma-\alpha-1} e^{zt} dt, \quad (5.62)$$

$$H_\nu(z) = \frac{1}{\Gamma(-\nu)} \int_0^\infty e^{-t^2 - 2zt} t^{-\nu-1} dt. \quad (5.63)$$

Here  $\text{Re } \gamma > \text{Re } \alpha > 0$  and  $\text{Re } (-\nu) > 0$ . These functions satisfy equations (5.49)–(5.51), respectively.

The Bessel equation is

$$z^2 u'' + zu' + (z^2 - \nu^2) u = 0, \quad (5.64)$$

where  $z$  is a complex variable and parameter  $\nu$  can have any real or complex values. The solutions of (5.64) are Bessel functions  $u_\nu(z)$  of order  $\nu$ . With the aid of the change of the function  $u = \varphi(z)y$  when  $\varphi(z) = z^\nu e^{iz}$  equation (5.64) can be reduced to the hypergeometric form

$$zy'' + (2iz + 2\nu + 1)y' + i(2\nu + 1)y = 0 \quad (5.65)$$

and based on Theorem 2 one can obtain the *Poisson integral representations* for the Bessel function of the first kind,  $J_\nu(z)$ , and the Hankel functions of the first and second kind,  $H_\nu^{(1)}(z)$  and  $H_\nu^{(2)}(z)$ :

$$J_\nu(z) = \frac{(z/2)^\nu}{\sqrt{\pi} \Gamma(\nu + 1/2)} \int_{-1}^1 (1 - t^2)^{\nu-1/2} \cos zt dt, \quad (5.66)$$

$$H_\nu^{(1,2)}(z) = \sqrt{\frac{2}{\pi z}} \frac{e^{\pm i(z - \pi\nu/2 - \pi/4)}}{\Gamma(\nu + 1/2)} \int_0^\infty e^{-t} t^{\nu-1/2} \left(1 \pm \frac{it}{2z}\right)^{\nu-1/2} dt, \quad (5.67)$$



where  $\text{Re } \nu > -1/2$ . It is then possible to deduce from these integral representations all the remaining properties of these functions. For details, see [57].

The Lommel equation

$$v'' + \frac{1-2\alpha}{\xi} v' + \left[ (\beta\gamma\xi^{\gamma-1})^2 + \frac{\alpha^2 - \nu^2\gamma^2}{\xi^2} \right] v = 0, \quad (5.68)$$

where  $\alpha$ ,  $\beta$  and  $\gamma$  some constants, is very convenient in applications. Its solutions are

$$v(\xi) = \xi^\alpha u_\nu(\beta\xi^\gamma), \quad (5.69)$$

where  $u_\nu(z)$  is a Bessel function of order  $\nu$ .

## 6. SOLUTION OF DIRAC WAVE EQUATION FOR COULOMB POTENTIAL

This section is written for the benefits of the reader who is not an expert in relativistic quantum mechanics and quantum field theory. We separate the variables and construct exact solutions of the Dirac equation of in spherical coordinates for the Coulomb field. The corresponding four component (bispinor) wave functions are given explicitly by (4.11)–(4.15). We first construct the angular parts of these solutions in terms of the so-called spinor spherical harmonics or spherical spinors.

**6.1. The Spinor Spherical Harmonics.** The vector addition  $\mathbf{j} = \mathbf{l} + \mathbf{s}$  of the orbital  $\mathbf{l} = -i\mathbf{r} \times \nabla$  and the spin  $\mathbf{s} = \frac{1}{2}\boldsymbol{\sigma}$  angular momenta (in the units of  $\hbar$ ) for the electron in the central field gives the eigenfunctions of the total angular momentum  $\mathbf{j}$ , or the spinor spherical harmonics [80], in the form

$$\mathcal{Y}_{jm}^{(l)}(\mathbf{n}) = \sum_{m_l+m_s=m} C_{lm_l \frac{1}{2}m_s}^{jm} Y_{lm_l}(\mathbf{n}) \chi_{\frac{1}{2}m_s} \quad (6.1)$$

$$(j = |l - 1/2|, l + 1/2; \quad m = -j, -j + 1, \dots, j - 1, j)$$

where  $Y_{lm}(\mathbf{n})$  with  $\mathbf{n} = \mathbf{n}(\theta, \varphi) = \mathbf{r}/r$  are the spherical harmonics,  $C_{lm_l \frac{1}{2}m_s}^{jm}$  are the special Clebsch-Gordan coefficients, and  $\chi_{m_s} = \chi_{\frac{1}{2}m_s}$  are eigenfunctions of the spin  $1/2$  operator  $\mathbf{s}$ :

$$\mathbf{s}^2 \chi_{\frac{1}{2}m_s} = \frac{3}{4} \chi_{\frac{1}{2}m_s}, \quad s_3 \chi_{\frac{1}{2}m_s} = m_s \chi_{\frac{1}{2}m_s}, \quad m_s = \pm 1/2 \quad (6.2)$$

given by

$$\chi_{\frac{1}{2}} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \chi_{-\frac{1}{2}} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}; \quad (6.3)$$

see [51], [63], [55], and [80]. From (6.1)

$$\begin{aligned} \mathcal{Y}_{jm}^{(l)}(\mathbf{n}) &= \sum_{m_s=-1/2}^{1/2} C_{l, m-m_s, \frac{1}{2}m_s}^{jm} Y_{l, m-m_s}(\mathbf{n}) \chi_{m_s} \\ &= C_{l, m+\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}}^{jm} Y_{l, m+\frac{1}{2}}(\mathbf{n}) \chi_{-\frac{1}{2}} + C_{l, m-\frac{1}{2}, \frac{1}{2}, \frac{1}{2}}^{jm} Y_{l, m-\frac{1}{2}}(\mathbf{n}) \chi_{\frac{1}{2}} \\ &= \begin{pmatrix} C_{l, m-\frac{1}{2}, \frac{1}{2}, \frac{1}{2}}^{jm} Y_{l, m-\frac{1}{2}}(\mathbf{n}) \\ C_{l, m+\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}}^{jm} Y_{l, m+\frac{1}{2}}(\mathbf{n}) \end{pmatrix}, \quad l = j \pm 1/2. \end{aligned} \quad (6.4)$$

Substituting the special values of the Clebsch–Gordan coefficients [80], we obtain the spinor spherical harmonics  $\mathcal{Y}_{jm}^\pm(\mathbf{n}) = \mathcal{Y}_{jm}^{(j\pm 1/2)}(\mathbf{n})$  in the form

$$\mathcal{Y}_{jm}^\pm(\mathbf{n}) = \begin{pmatrix} \mp \sqrt{\frac{(j+1/2) \mp (m-1/2)}{2j+(1\pm 1)}} Y_{j\pm 1/2, m-1/2}(\mathbf{n}) \\ \sqrt{\frac{(j+1/2) \pm (m+1/2)}{2j+(1\pm 1)}} Y_{j\pm 1/2, m+1/2}(\mathbf{n}) \end{pmatrix} \quad (6.5)$$

with the total angular momentum  $j = 1/2, 3/2, 5/2, \dots$  and its projection  $m = -j, -j+1, \dots, j-1, j$ . The orthogonality property for the spinor spherical harmonics  $\mathcal{Y}_{jm}^\pm(\mathbf{n}) = \mathcal{Y}_{jm}^{(j\pm 1/2)}(\mathbf{n})$  is [80]

$$\int_{S^2} \left( \mathcal{Y}_{jm}^{(l)}(\mathbf{n}) \right)^\dagger \mathcal{Y}_{j'm'}^{(l')}(\mathbf{n}) d\omega = \delta_{jj'} \delta_{ll'} \delta_{mm'} \quad (6.6)$$

with  $d\omega = \sin \theta d\theta d\varphi$  and  $0 \leq \theta \leq \pi, 0 \leq \varphi \leq 2\pi$ . They are common eigenfunctions of the following set of commuting operators

$$\mathbf{j}^2 \mathcal{Y}_{jm}^\pm(\mathbf{n}) = \left( \mathbf{l} + \frac{1}{2} \boldsymbol{\sigma} \right)^2 \mathcal{Y}_{jm}^\pm(\mathbf{n}) = j(j+1) \mathcal{Y}_{jm}^\pm(\mathbf{n}), \quad (6.7)$$

$$j_3 \mathcal{Y}_{jm}^\pm(\mathbf{n}) = m \mathcal{Y}_{jm}^\pm(\mathbf{n}), \quad (6.8)$$

$$\mathbf{l}^2 \mathcal{Y}_{jm}^\pm(\mathbf{n}) = \left( j \pm \frac{1}{2} \right) \left( j \pm \frac{1}{2} + 1 \right) \mathcal{Y}_{jm}^\pm(\mathbf{n}), \quad (6.9)$$

$$\boldsymbol{\sigma}^2 \mathcal{Y}_{jm}^\pm(\mathbf{n}) = 3 \mathcal{Y}_{jm}^\pm(\mathbf{n}). \quad (6.10)$$

But

$$\mathbf{j}^2 = \left( \mathbf{l} + \frac{1}{2} \boldsymbol{\sigma} \right)^2 = \mathbf{l}^2 + \boldsymbol{\sigma} \cdot \mathbf{l} + \frac{3}{4},$$

or

$$\boldsymbol{\sigma} \cdot \mathbf{l} = \mathbf{j}^2 - \mathbf{l}^2 - \frac{3}{4}. \quad (6.11)$$

This implies that the spinor spherical harmonics  $\mathcal{Y}_{jm}^\pm(\mathbf{n})$  are also eigenfunctions of the operator  $\boldsymbol{\sigma} \cdot \mathbf{l}$ :

$$(\boldsymbol{\sigma} \cdot \mathbf{l}) \mathcal{Y}_{jm}^\pm(\mathbf{n}) = - \left( 1 \pm \left( j + \frac{1}{2} \right) \right) \mathcal{Y}_{jm}^\pm(\mathbf{n}), \quad (6.12)$$

and it is a custom to write

$$(\boldsymbol{\sigma} \cdot \mathbf{l}) \mathcal{Y}_{jm}^\pm(\mathbf{n}) = - (1 + \kappa) \mathcal{Y}_{jm}^\pm(\mathbf{n}), \quad (6.13)$$

where the quantum number  $\kappa = \kappa_\pm = \pm \left( j + \frac{1}{2} \right) = \pm 1, \pm 2, \pm 3, \dots$  takes all positive and negative integer values with exception of zero:  $\kappa \neq 0$ .

Finally, the following relation for the spinor spherical harmonics,

$$(\boldsymbol{\sigma} \cdot \mathbf{n}) \mathcal{Y}_{jm}^\pm(\mathbf{n}) = - \mathcal{Y}_{jm}^\mp(\mathbf{n}), \quad (6.14)$$

plays an important role in the Dirac theory of relativistic electron. In view of  $(\boldsymbol{\sigma} \cdot \mathbf{n})^2 = \mathbf{1}$ , it is sufficient to prove only one of these relations, say

$$(\boldsymbol{\sigma} \cdot \mathbf{n}) \mathcal{Y}_{jm}^+(\mathbf{n}) = - \mathcal{Y}_{jm}^-(\mathbf{n}),$$

and the second will follow. A direct proof can be given by using the recurrence relations for the spherical harmonics (8.17)–(8.19), or with the help of the Wigner–Eckart theorem; see [63] and [80], the reader can work out the details.

The quadratic forms

$$Q_{jm} = \left( \mathcal{Y}_{jm}^{(l)}(\mathbf{n}) \right)^\dagger \mathcal{Y}_{jm}^{(l)}(\mathbf{n}) \quad (6.15)$$

of the spinor spherical harmonics  $\mathcal{Y}_{jm}^{(l)}(\mathbf{n})$  describe the angular distributions of the electron in states with the total angular momentum  $j$ , its projection  $m$  and the orbital angular momentum  $l$ . These forms, given by [80]

$$\begin{aligned} Q_{jm}(\theta) &= \frac{1}{2j} \left( (j+m) |Y_{j-1/2, m-1/2}(\mathbf{n})|^2 + (j-m) |Y_{j-1/2, m+1/2}(\mathbf{n})|^2 \right) \\ &= \frac{1}{2j+2} \left( (j+m+1) |Y_{j+1/2, m+1/2}(\mathbf{n})|^2 + (j-m+1) |Y_{j+1/2, m-1/2}(\mathbf{n})|^2 \right), \end{aligned} \quad (6.16)$$

are, in fact, independent of  $l$  and  $\varphi$ . There is the useful expansion in terms of the Laguerre polynomials

$$Q_{jm}(\theta) = \sum_{s=0}^{j-1/2} a_s(j, m) P_{2s}(\cos \theta) \quad (6.17)$$

with the coefficients of the form

$$\begin{aligned} a_s(j, m) &= -\frac{4s+1}{4\pi} \sqrt{2j(2j+1)} \left\{ \begin{matrix} j & j & 2s \\ j-1/2 & j-1/2 & 1/2 \end{matrix} \right\} C_{j-1/2, 0, 2s0}^{j-1/2, 0} C_{jm \ 2s0}^{jm} \\ &= (-1)^s \frac{4s+1}{4\pi} \sqrt{\frac{(2j+2s+1)(2j-2s)!}{(2j+1)(2j+2s)!}} \frac{(j+s-1/2)!(2s)!}{(j-s-1/2)!(s!)^2} C_{jm \ 2s0}^{jm}. \end{aligned} \quad (6.18)$$

See [80] for more information.

**6.2. Separation of Variables in Spherical Coordinates.** Using the explicit form of the  $\alpha$  and  $\beta$  matrices (4.3) we rewrite the stationary Dirac equation (4.9) in a central field with the Hamiltonian

$$H = c\alpha\mathbf{p} + mc^2\beta + U(r) = \begin{pmatrix} U + mc^2 & c\sigma\mathbf{p} \\ c\sigma\mathbf{p} & U - mc^2 \end{pmatrix} \quad (6.19)$$

and the bispinor wave function

$$\psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix} \quad (6.20)$$

in a matrix form

$$\begin{pmatrix} U + mc^2 & c\sigma\mathbf{p} \\ c\sigma\mathbf{p} & U - mc^2 \end{pmatrix} \begin{pmatrix} \varphi \\ \chi \end{pmatrix} = E \begin{pmatrix} \varphi \\ \chi \end{pmatrix}, \quad (6.21)$$

or

$$c\sigma\mathbf{p} \varphi = (E + mc^2 - U) \chi, \quad (6.22)$$

$$c\sigma\mathbf{p} \chi = (E - mc^2 - U) \varphi. \quad (6.23)$$

Here we shall use the following operator identity

$$\sigma \cdot \nabla = (\sigma \cdot \mathbf{n}) (\mathbf{n} \cdot \nabla + i\sigma \cdot (\mathbf{n} \times \nabla)) \quad (6.24)$$

in the form

$$c\boldsymbol{\sigma}\mathbf{p} = \hbar c (\boldsymbol{\sigma}\mathbf{n}) \left( \frac{1}{i} \mathbf{n} \boldsymbol{\nabla} + \frac{i}{r} \boldsymbol{\sigma} \mathbf{l} \right), \quad (6.25)$$

where  $\mathbf{l} = -i\mathbf{r} \times \boldsymbol{\nabla}$  is the operator of orbital angular momentum,  $\mathbf{n} = \mathbf{r}/r$  and  $\mathbf{p} = -i\hbar\boldsymbol{\nabla}$ . It can be obtained as a consequence of a more general operator identity [31]

$$(\boldsymbol{\sigma} \cdot \mathbf{A}) (\boldsymbol{\sigma} \cdot \mathbf{B}) = \mathbf{A} \cdot \mathbf{B} + i\boldsymbol{\sigma} \cdot (\mathbf{A} \times \mathbf{B}), \quad (6.26)$$

which is valid for any vector operators  $\mathbf{A}$  and  $\mathbf{B}$  commuting with the Pauli  $\boldsymbol{\sigma}$ -matrices; it is not required that  $\mathbf{A}$  and  $\mathbf{B}$  commute. The proof uses a familiar property of the Pauli matrices

$$\sigma_i \sigma_k = i e_{ikl} \sigma_l + \delta_{ik}, \quad (6.27)$$

where  $e_{ikl}$  is the completely antisymmetric Levi-Civita symbol,  $\delta_{ik}$  is the symmetric Kronecker delta symbol and we use Einstein's summation rule over the repeating indices; it is understood that a summation is to be taken over the three values of  $l = 1, 2, 3$ . Thus

$$\begin{aligned} (\boldsymbol{\sigma} \cdot \mathbf{A}) (\boldsymbol{\sigma} \cdot \mathbf{B}) &= (\sigma_i A_i) (\sigma_k B_k) \\ &= (\sigma_i \sigma_k) A_i B_k = i\sigma_l e_{ikl} A_i B_k + \delta_{ik} A_i B_k \\ &= i\sigma_l (\mathbf{A} \times \mathbf{B})_l + A_k B_k = i\boldsymbol{\sigma} \cdot (\mathbf{A} \times \mathbf{B}) + \mathbf{A} \cdot \mathbf{B}, \end{aligned}$$

where  $(\mathbf{A} \times \mathbf{B})_l = e_{lik} A_i B_k = e_{ikl} A_i B_k$  in view of antisymmetry of the Levi-Civita symbol:  $e_{ikl} = -e_{ilk} = e_{lik}$ , and  $\delta_{ik} A_i = A_k$ .

If  $\mathbf{A} = \mathbf{B}$ , Eq. (6.26) implies  $(\boldsymbol{\sigma} \cdot \mathbf{A})^2 = \mathbf{A}^2$ . In particular,  $(\boldsymbol{\sigma}\mathbf{n})^2 = \mathbf{n}^2 = \mathbf{1}$ , and the proof of the “gradient” formula (6.24) is

$$\begin{aligned} \boldsymbol{\sigma} \cdot \boldsymbol{\nabla} &= (\boldsymbol{\sigma} \cdot \mathbf{n})^2 (\boldsymbol{\sigma} \cdot \boldsymbol{\nabla}) = (\boldsymbol{\sigma} \cdot \mathbf{n}) ((\boldsymbol{\sigma} \cdot \mathbf{n}) (\boldsymbol{\sigma} \cdot \boldsymbol{\nabla})) \\ &= (\boldsymbol{\sigma} \cdot \mathbf{n}) (\mathbf{n} \cdot \boldsymbol{\nabla} + i\boldsymbol{\sigma} \cdot (\mathbf{n} \times \boldsymbol{\nabla})) \end{aligned}$$

by (6.26) with  $\mathbf{A} = \mathbf{n}$  and  $\mathbf{B} = \boldsymbol{\nabla}$ . In a similar fashion, one can derive the following “anticommutation” relation,

$$(\boldsymbol{\sigma}\mathbf{n}) (\boldsymbol{\sigma}\mathbf{l}) + (\boldsymbol{\sigma}\mathbf{l}) (\boldsymbol{\sigma}\mathbf{n}) = -2(\boldsymbol{\sigma}\mathbf{n}), \quad \mathbf{n} = \mathbf{r}/r, \quad (6.28)$$

we leave details to the reader.

The structure of operator  $\boldsymbol{\sigma}\mathbf{p}$  in (6.25) suggests to look for solutions of the Dirac system (6.22)–(6.23) in spherical coordinates  $\mathbf{r} = r \mathbf{n}(\theta, \varphi)$  in the form of the Ansatz:

$$\boldsymbol{\varphi} = \boldsymbol{\varphi}(\mathbf{r}) = \mathcal{Y}(\mathbf{n}) F(r), \quad (6.29)$$

$$\boldsymbol{\chi} = \boldsymbol{\chi}(\mathbf{r}) = -i((\boldsymbol{\sigma}\mathbf{n}) \mathcal{Y}(\mathbf{n})) G(r), \quad (6.30)$$

where  $\mathcal{Y} = \mathcal{Y}_{jm}^{\pm}(\mathbf{n})$  are the spinor spherical harmonics given by (6.5). This substitution preserves the symmetry properties of the wave functions under inversion  $\mathbf{r} \rightarrow -\mathbf{r}$ . Then the radial functions  $F(r)$  and  $G(r)$  satisfy the system of two first order ordinary differential equations

$$\frac{dF}{dr} + \frac{1+\kappa}{r} F = \frac{mc^2 + E - U(r)}{\hbar c} G, \quad (6.31)$$

$$\frac{dG}{dr} + \frac{1-\kappa}{r} G = \frac{mc^2 - E + U(r)}{\hbar c} F, \quad (6.32)$$

where  $\kappa = \kappa_{\pm} = \pm(j + 1/2) = \pm 1, \pm 2, \pm 3, \dots$ , respectively.

If  $f = f(\mathbf{r}) = f(r\mathbf{n})$ , then

$$\frac{\partial f}{\partial r} = \frac{\partial f}{\partial \mathbf{r}} \frac{\partial \mathbf{r}}{\partial r} = \mathbf{n} \nabla f$$

and in spherical coordinates Eq. (6.25) becomes

$$c\boldsymbol{\sigma}\mathbf{p} = \hbar c(\boldsymbol{\sigma}\mathbf{n}) \left( \frac{1}{i} \frac{\partial}{\partial r} + \frac{i}{r} \boldsymbol{\sigma}\mathbf{l} \right). \quad (6.33)$$

Thus

$$\begin{aligned} c\boldsymbol{\sigma}\mathbf{p} \varphi &= \hbar c(\boldsymbol{\sigma}\mathbf{n}) \left( \frac{1}{i} \frac{\partial}{\partial r} + \frac{i}{r} \boldsymbol{\sigma}\mathbf{l} \right) \mathcal{Y}F \\ &= \hbar c(\boldsymbol{\sigma}\mathbf{n}) \left( \frac{1}{i} \mathcal{Y} \frac{dF}{dr} + \frac{i}{r} (\boldsymbol{\sigma}\mathbf{l}\mathcal{Y}) F \right) \\ &= -i\hbar c(\boldsymbol{\sigma}\mathbf{n}\mathcal{Y}) \left( \frac{dF}{dr} + \frac{1+\kappa}{r} F \right) \end{aligned}$$

by (6.13), and we arrive at (6.31) in view of (6.22) and (6.30). Equation (6.32) can be verified in a similar fashion with the help of (6.28) or (6.14).

Eqs. (6.31)–(6.32) hold in any central field with the potential energy  $U = U(r)$ . For states with discrete spectra the radial functions  $rF(r)$  and  $rG(r)$  should be bounded as  $r \rightarrow 0$  and satisfy the normalization condition

$$\int_{\mathbf{R}^3} \psi^\dagger \psi \, dv = \int_0^\infty r^2 (F^2(r) + G^2(r)) \, dr = 1 \quad (6.34)$$

in view of (4.7), (6.29)–(6.30) and (6.6).

**6.3. Solution of Radial Equations.** For the relativistic Coulomb problem  $U = -Ze^2/r$ , we introduce the dimensionless quantities

$$\varepsilon = \frac{E}{mc^2}, \quad x = \beta r = \frac{mc}{\hbar} r, \quad \mu = \frac{Ze^2}{\hbar c} \quad (6.35)$$

and the radial functions

$$f(x) = F(r), \quad g(x) = G(r). \quad (6.36)$$

The system (6.31)–(6.32) becomes

$$\frac{df}{dx} + \frac{1+\kappa}{x} f = \left( 1 + \varepsilon + \frac{\mu}{x} \right) g, \quad (6.37)$$

$$\frac{dg}{dx} + \frac{1-\kappa}{x} g = \left( 1 - \varepsilon - \frac{\mu}{x} \right) f. \quad (6.38)$$

We shall see later that in nonrelativistic limit  $c \rightarrow \infty$  the following estimate holds  $|f(x)| \gg |g(x)|$ .

We follow [57] with somewhat different details. Let us rewrite the system (6.37)–(6.38) in matrix form [43]. If

$$u = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \begin{pmatrix} xf(x) \\ xg(x) \end{pmatrix}, \quad u' = \begin{pmatrix} u'_1 \\ u'_2 \end{pmatrix}. \quad (6.39)$$

Then

$$u' = Au, \quad (6.40)$$

where

$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} = \begin{pmatrix} -\frac{\kappa}{x} & 1 + \varepsilon + \frac{\mu}{x} \\ 1 - \varepsilon - \frac{\mu}{x} & \frac{\kappa}{x} \end{pmatrix}. \quad (6.41)$$

To find  $u_1(x)$ , we eliminate  $u_2(x)$  from the system (6.40), obtaining a second order differential equation

$$\begin{aligned} u_1'' - \left( a_{11} + a_{22} + \frac{a'_{12}}{a_{12}} \right) u_1' \\ + \left( a_{11}a_{22} - a_{12}a_{21} - a'_{11} + \frac{a'_{12}}{a_{12}} a_{11} \right) u_1 = 0. \end{aligned} \quad (6.42)$$

Similarly, eliminating  $u_1(x)$ , one gets equation for  $u_2(x)$ :

$$\begin{aligned} u_2'' - \left( a_{11} + a_{22} + \frac{a'_{21}}{a_{21}} \right) u_2' \\ + \left( a_{11}a_{22} - a_{12}a_{21} - a'_{22} + \frac{a'_{21}}{a_{21}} a_{22} \right) u_2 = 0. \end{aligned} \quad (6.43)$$

The components of matrix  $A$  have the form

$$a_{ik} = b_{ik} + c_{ik}/x, \quad (6.44)$$

where  $b_{ik}$  and  $c_{ik}$  are constants. Equations (6.42) and (6.43) are not generalized equations of hypergeometric type (5.1). Indeed,

$$\frac{a'_{12}}{a_{12}} = -\frac{c_{12}}{c_{12}x + b_{12}x^2},$$

and the coefficients of  $u_1'(x)$  and  $u_1(x)$  in (6.42) are

$$\begin{aligned} a_{11} + a_{22} + \frac{a'_{12}}{a_{12}} &= \frac{p_1(x)}{x} - \frac{c_{12}}{c_{12}x + b_{12}x^2}, \\ a_{11}a_{22} - a_{12}a_{21} - a'_{11} + \frac{a'_{12}}{a_{12}}a_{11} &= \frac{p_2(x)}{x^2} - \frac{c_{12}(c_{11} + b_{11}x)}{(c_{12} + b_{12}x)x^2}, \end{aligned}$$

where  $p_1(x)$  and  $p_2(x)$  are polynomials of degrees at most one and two, respectively. Equation (6.42) will become a generalized equation of hypergeometric type (5.1) with  $\sigma(x) = x$  if either  $b_{12} = 0$  or  $c_{12} = 0$ . The following consideration helps. By a linear transformation

$$\begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = C \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} \quad (6.45)$$

with a nonsingular matrix  $C$  that is independent of  $x$  we transform the original system (6.40) to a similar one

$$v' = \tilde{A}v, \quad (6.46)$$

where

$$v = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}, \quad \tilde{A} = CAC^{-1} = \begin{pmatrix} \tilde{a}_{11} & \tilde{a}_{12} \\ \tilde{a}_{21} & \tilde{a}_{22} \end{pmatrix}.$$

The new coefficients  $\tilde{a}_{ik}$  are linear combinations of the original ones  $a_{ik}$ . Hence they have a similar form

$$\tilde{a}_{ik} = \tilde{b}_{ik} + \tilde{c}_{ik}/x, \quad (6.47)$$

where  $\tilde{b}_{ik}$  and  $\tilde{c}_{ik}$  are constants.

The equations for  $v_1(x)$  and  $v_2(x)$  are similar to (6.42) and (6.43):

$$\begin{aligned} v_1'' - \left( \tilde{a}_{11} + \tilde{a}_{22} + \frac{\tilde{a}_{12}'}{\tilde{a}_{12}} \right) v_1' \\ + \left( \tilde{a}_{11}\tilde{a}_{22} - \tilde{a}_{12}\tilde{a}_{21} - \tilde{a}_{11}' + \frac{\tilde{a}_{12}'}{\tilde{a}_{12}} \tilde{a}_{11} \right) v_1 = 0, \end{aligned} \quad (6.48)$$

$$\begin{aligned} v_2'' - \left( \tilde{a}_{11} + \tilde{a}_{22} + \frac{\tilde{a}_{21}'}{\tilde{a}_{21}} \right) v_2' \\ + \left( \tilde{a}_{11}\tilde{a}_{22} - \tilde{a}_{12}\tilde{a}_{21} - \tilde{a}_{22}' + \frac{\tilde{a}_{21}'}{\tilde{a}_{21}} \tilde{a}_{22} \right) v_2 = 0. \end{aligned} \quad (6.49)$$

The calculation of the coefficients in (6.48) and (6.49) is facilitated by a similarity of the matrices  $A$  and  $\tilde{A}$ :

$$\tilde{a}_{11} + \tilde{a}_{22} = a_{11} + a_{22}, \quad \tilde{a}_{11}\tilde{a}_{22} - \tilde{a}_{12}\tilde{a}_{21} = a_{11}a_{22} - a_{12}a_{21}.$$

By a previous consideration, in order for (6.48) to be an equation of hypergeometric type, it is sufficient to choose either  $\tilde{b}_{12} = 0$  or  $\tilde{c}_{12} = 0$ . Similarly, for (6.49): either  $\tilde{b}_{21} = 0$  or  $\tilde{c}_{21} = 0$ . These conditions impose certain restrictions on our choice of the transformation matrix  $C$ . Let

$$C = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}. \quad (6.50)$$

Then

$$C^{-1} = \frac{1}{\Delta} \begin{pmatrix} \delta & -\beta \\ -\gamma & \alpha \end{pmatrix}, \quad \Delta = \det C = \alpha\delta - \beta\gamma,$$

and

$$\begin{aligned} \tilde{A} &= CAC^{-1} \\ &= \frac{1}{\Delta} \begin{pmatrix} a_{11}\alpha\delta - a_{12}\alpha\gamma + a_{21}\beta\delta - a_{22}\beta\gamma & a_{12}\alpha^2 - a_{12}\beta^2 + (a_{22} - a_{11})\alpha\beta \\ a_{21}\delta^2 - a_{12}\gamma^2 + (a_{11} - a_{22})\gamma\delta & a_{12}\alpha\gamma - a_{11}\beta\gamma + a_{22}\alpha\delta - a_{21}\beta\delta \end{pmatrix}. \end{aligned} \quad (6.51)$$

For the Dirac system (6.40)–(6.41):

$$\begin{aligned} a_{11} &= -\frac{\kappa}{x}, & a_{12} &= 1 + \varepsilon + \frac{\mu}{x}, \\ a_{21} &= 1 - \varepsilon - \frac{\mu}{x}, & a_{22} &= \frac{\kappa}{x} \end{aligned}$$

and

$$\Delta \tilde{a}_{12} = \alpha^2 - \beta^2 + (\alpha^2 + \beta^2)\varepsilon + \frac{(\alpha^2 + \beta^2)\mu + 2\alpha\beta\kappa}{x}, \quad (6.52)$$

$$\Delta \tilde{a}_{21} = \delta^2 - \gamma^2 - (\delta^2 + \gamma^2)\varepsilon - \frac{(\delta^2 + \gamma^2)\mu + 2\gamma\delta\kappa}{x}. \quad (6.53)$$

$$\begin{array}{llll}
\text{The condition} & \tilde{b}_{12} = 0 & \text{yields} & (1 + \varepsilon) \alpha^2 - (1 - \varepsilon) \beta^2 = 0, \\
" & " & & \tilde{c}_{12} = 0 \quad " \quad (\alpha^2 + \beta^2) \mu + 2\alpha\beta\kappa = 0, \\
" & " & & \tilde{b}_{21} = 0 \quad " \quad (1 + \varepsilon) \gamma^2 - (1 - \varepsilon) \delta^2 = 0, \\
" & " & & \tilde{c}_{21} = 0 \quad " \quad (\delta^2 + \gamma^2) \mu + 2\gamma\delta\kappa = 0.
\end{array}$$

We see that there are several possibilities to choose the elements  $\alpha, \beta, \gamma, \delta$  of the transition matrix  $C$ . All quantum mechanics textbooks use the original one, namely,  $\tilde{b}_{12} = 0$  and  $\tilde{b}_{21} = 0$ , due to Darwin [30] and Gordon [43]; cf. equations (6.83)–(6.84) below. Nikiforov and Uvarov [57] take another path, they choose  $\tilde{c}_{12} = 0$  and  $\tilde{c}_{21} = 0$  and show that it is more convenient for taking the nonrelativistic limit  $c \rightarrow \infty$ . These conditions are satisfied if

$$C = \begin{pmatrix} \mu & \nu - \kappa \\ \nu - \kappa & \mu \end{pmatrix}, \quad (6.54)$$

where  $\nu = \sqrt{\kappa^2 - \mu^2}$ , and we finally arrive at the following system of the first order equations for  $v_1(x)$  and  $v_2(x)$ :

$$v_1' = \left( \frac{\varepsilon\mu}{\nu} - \frac{\nu}{x} \right) v_1 + \left( 1 + \frac{\varepsilon\kappa}{\nu} \right) v_2, \quad (6.55)$$

$$v_2' = \left( 1 - \frac{\varepsilon\kappa}{\nu} \right) v_1 + \left( \frac{\nu}{x} - \frac{\varepsilon\mu}{\nu} \right) v_2. \quad (6.56)$$

Here

$$\text{Tr } \tilde{A} = \tilde{a}_{11} + \tilde{a}_{22} = 0, \quad \det \tilde{A} = \varepsilon^2 - 1 + \frac{2\varepsilon\mu}{x} - \frac{\nu^2}{x^2}, \quad \nu^2 = \kappa^2 - \mu^2, \quad (6.57)$$

which is simpler than the original choice in [57]. The corresponding second order differential equations (6.48)–(6.49) become

$$v_1'' + \frac{(\varepsilon^2 - 1)x^2 + 2\varepsilon\mu x - \nu(\nu + 1)}{x^2} v_1 = 0, \quad (6.58)$$

$$v_2'' + \frac{(\varepsilon^2 - 1)x^2 + 2\varepsilon\mu x - \nu(\nu - 1)}{x^2} v_2 = 0. \quad (6.59)$$

They are the generalized equations of hypergeometric type (5.1) of a simplest form  $\tilde{\tau} = 0$ , thus resembling the one dimensional Schrödinger equation; the second equation can be obtained from the first one by replacing  $\nu \rightarrow -\nu$ .

Let  $1 + \varepsilon\kappa/\nu = 0$ , then  $\varepsilon = -\nu/\kappa$  that is possible only if  $\kappa < 0$ , since  $\nu > 0$  and  $\varepsilon > 0$ . The corresponding solution of (6.55),

$$v_1(x) = C_1 x^{-\nu} e^{(\varepsilon\mu x)/\nu},$$

satisfies the conditions of the problem only if  $C_1 = 0$ . Then from (6.56)

$$v_2(x) = C_2 x^\nu e^{-(\varepsilon\mu x)/\nu},$$

which does satisfy the condition of the problem with  $C_2 \neq 0$ .

Let us analyze the behavior of the solutions of (6.58) as  $x \rightarrow 0$ . Since

$$|(\varepsilon^2 - 1)x^2 + 2\varepsilon\mu x| \ll \nu(\nu + 1)$$

as  $x \rightarrow 0$ , one can approximate this equation in the neighborhood of  $x = 0$  by the corresponding Euler equation

$$x^2 v_1'' - \nu(\nu + 1) v_1 = 0,$$



whose solutions are

$$v_1(x) = C_1 x^{\nu+1} + C_2 x^{-\nu}, \quad C_2 = 0.$$

Thus  $v_1 \rightarrow C_1 x^{\nu+1}$  as  $x \rightarrow 0$ . The results for (6.59) are similar:  $v_2 \rightarrow C_2 x^{-\nu}$  as  $x \rightarrow 0$ ; one can use the symmetry  $\nu \rightarrow -\nu$ .

Equation (6.58) is the generalized equation of hypergeometric type (5.1) with

$$\begin{aligned} \sigma(x) &= x, & \tilde{\tau}(x) &= 0, \\ \tilde{\sigma}(x) &= (\varepsilon^2 - 1)x^2 + 2\varepsilon\mu x - \nu(\nu + 1). \end{aligned}$$

The substitution

$$v_1 = \varphi(x) y(x), \quad \frac{\varphi'}{\varphi} = \frac{\pi(x)}{\sigma(x)}, \quad (6.60)$$

where

$$\pi(x) = \frac{\sigma' - \tilde{\tau}}{2} \pm \sqrt{\left(\frac{\sigma' - \tilde{\tau}}{2}\right)^2 - \tilde{\sigma} + k\sigma} \quad (6.61)$$

with  $k = \lambda - \pi'$  and  $\tau(x) = \tilde{\tau}(x) + 2\pi(x)$ , results in the equation of hypergeometric type

$$\sigma(x) y'' + \tau(x) y' + \lambda y = 0 \quad (6.62)$$

by the method of [57]; see also Section 5.1. From the four possible forms of  $\pi(x)$ :

$$\pi(x) = \frac{1}{2} \pm \left( \sqrt{1 - \varepsilon^2} x \pm \left( \nu + \frac{1}{2} \right) \right), \quad (6.63)$$

corresponding to the values of  $k$  determined by the condition of the zero discriminant of the quadratic polynomial under the square root sign in (6.61):

$$k - 2\varepsilon\mu = \pm \sqrt{1 - \varepsilon^2} (2\nu + 1), \quad (6.64)$$

we select the one when the function  $\tau(x)$  has a negative derivative and a zero on  $(0, +\infty)$ . This is true if one chooses

$$\begin{aligned} k &= 2\varepsilon\mu - a(2\nu + 1), \\ \pi(x) &= \nu + 1 - ax, \\ \tau(x) &= 2\pi(x) = 2(\nu + 1 - ax), \\ \lambda &= k + \pi' = 2(\varepsilon\mu - a(\nu + 1)) \end{aligned}$$

and

$$\varphi(x) = x^{\nu+1} e^{-ax}, \quad \rho(x) = x^{2\nu+1} e^{-2ax},$$

where  $a = \sqrt{1 - \varepsilon^2}$  and  $\nu = \sqrt{\kappa^2 - \mu^2}$ . The analysis for (6.59) is similar, one can use the symmetry  $\nu \rightarrow -\nu$  in (6.63)–(6.64).

From (6.34) and (6.39)

$$\int_0^\infty r^2 (F^2(r) + G^2(r)) dr = \beta^{-3} \int_0^\infty (u_1^2(x) + u_2^2(x)) dx = 1. \quad (6.65)$$

It requires by (6.45) the square integrability of  $v_1(x)$  and  $v_2(x)$ . Their boundness at  $x = 0$  follows from the asymptotic behavior as  $x \rightarrow 0$ . So

$$\int_0^\infty v_1^2(x) dx = \int_0^\infty \varphi^2(x) y^2(x) dx = \int_0^\infty x y^2(x) \rho(x) dx < \infty. \quad (6.66)$$

For the time being, we replace this condition by

$$\int_0^\infty y^2(x) \rho(x) dx < \infty \quad (6.67)$$

in order to apply Theorem 1, and will verify the normalization condition (6.65) later. Then the corresponding energy levels  $\varepsilon = \varepsilon_n$  are determined by

$$\lambda + n\tau' + \frac{1}{2}n(n-1)\sigma'' = 0 \quad (n = 0, 1, 2, \dots), \quad (6.68)$$

whence

$$\varepsilon\mu = a(\nu + n + 1), \quad (6.69)$$

and the eigenfunctions are given by the Rodrigues formula

$$y_n(x) = \frac{C_n}{\rho(x)} (\sigma^n(x) \rho(x))^{(n)} = C_n x^{-2\nu-1} e^{2ax} \frac{d^n}{dx^n} (x^{2\nu+n+1} e^{-2ax}). \quad (6.70)$$

The functions  $y_n(x)$  are, up to certain constants, the Laguerre polynomials  $L_n^{2\nu+1}(\xi)$  with  $\xi = 2ax$ .

The previously found eigenvalue  $\varepsilon = -\nu/\kappa$  satisfies (6.69) with  $n = -1$ . Consequently it is natural to replace  $n$  by  $n - 1$  in (6.69)–(6.70) and define the eigenvalues by

$$\varepsilon\mu = a(\nu + n), \quad a = \sqrt{1 - \varepsilon^2} \quad (n = 0, 1, 2, \dots). \quad (6.71)$$

Solving for  $\varepsilon$  gives the Sommerfeld–Dirac formula (4.16). The corresponding eigenfunctions have the form

$$v_1(x) = \begin{cases} 0, & n = 0, \\ A_n \xi^{\nu+1} e^{-\xi/2} L_{n-1}^{2\nu+1}(\xi), & n = 1, 2, 3, \dots \end{cases} \quad (6.72)$$

They are square integrable functions on  $(0, \infty)$ . The counterparts are

$$v_2(x) = B_n \xi^\nu e^{-\xi/2} L_n^{2\nu-1}(\xi), \quad n = 0, 1, 2, \dots \quad (6.73)$$

It is easily seen that our previous solution for  $\varepsilon = -\nu/\kappa$  is included in this formula when  $n = 0$ . By equation (6.55) the other solutions can be obtain as

$$v_2(x) = \frac{1}{1 + \kappa\varepsilon/\nu} \left( v_1'(x) + \left( \frac{\nu}{x} - \frac{\varepsilon\mu}{\nu} \right) v_1(x) \right)$$

and substituting  $v_1(x)$  from (6.72) one gets

$$v_2(x) = \xi^\nu e^{-\xi/2} Y(\xi),$$

where  $Y(\xi)$  is a polynomial of degree  $n$ . But function  $v_2(x)$  satisfies (6.59). By the previous consideration the substitution

$$v_2(x) = x^\nu e^{-ax} y(x)$$

gives

$$xy'' + (2\nu - 2ax)y' + 2any = 0,$$

in view of the quantization rule (6.71). The change of the variable  $y(x) = Y(\xi)$  with  $\xi = 2ax$  results in

$$\xi Y'' + (2\nu - \xi)Y' + nY = 0 \quad (6.74)$$

and the only polynomial solutions are the Laguerre polynomials  $L_n^{2\nu-1}(\xi)$ , whence (6.73) is correct. Solutions  $v_2(x)$  are square integrable functions on  $(0, \infty)$ .

To find the relations between the coefficients  $A_n$  and  $B_n$  in (6.72) and (6.73) we take the limit  $x \rightarrow 0$  in (6.55) with the help of the following properties of the Laguerre polynomials [55], [57], [74]:

$$\frac{d}{d\xi} L_n^\alpha(\xi) = -L_{n-1}^{\alpha+1}(\xi), \quad L_n^\alpha(0) = \frac{\Gamma(\alpha + n + 1)}{n! \Gamma(\alpha + 1)}. \quad (6.75)$$

The result is

$$2a(\nu + 1) A_n L_{n-1}^{2\nu+1}(0) = -2a\nu A_n L_{n-1}^{2\nu+1}(0) + \left(1 + \frac{\varepsilon\kappa}{\nu}\right) B_n L_n^{2\nu-1}(0),$$

whence

$$A_n = \frac{\nu + \varepsilon\kappa}{an(n + 2\nu)} B_n \quad (n = 1, 2, 3, \dots).$$

Since

$$\begin{aligned} a^2 n(n + 2\nu) &= a^2 ((n + \nu)^2 - \nu^2) = \mu^2 \varepsilon^2 - a^2 \nu^2 \\ &= \mu^2 \varepsilon^2 - (1 - \varepsilon^2) \nu^2 = \kappa^2 \varepsilon^2 - \nu^2, \end{aligned}$$

we have proved the useful identity

$$a^2 n(n + 2\nu) = \varepsilon^2 \kappa^2 - \nu^2, \quad (6.76)$$

and the final relation is

$$A_n = \frac{a}{\kappa\varepsilon - \nu} B_n. \quad (6.77)$$

By (6.45) and (6.54) we find

$$\begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = C^{-1} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}, \quad C^{-1} = \frac{1}{2\nu(\kappa - \nu)} \begin{pmatrix} \mu & \kappa - \nu \\ \kappa - \nu & \mu \end{pmatrix}.$$

Therefore

$$xf(x) = \frac{B_n}{2\nu(\kappa - \nu)} \xi^\nu e^{-\xi/2} (f_1 \xi L_{n-1}^{2\nu+1}(\xi) + f_2 L_n^{2\nu-1}(\xi)), \quad (6.78)$$

$$xg(x) = \frac{B_n}{2\nu(\kappa - \nu)} \xi^\nu e^{-\xi/2} (g_1 \xi L_{n-1}^{2\nu+1}(\xi) + g_2 L_n^{2\nu-1}(\xi)), \quad (6.79)$$

where

$$f_1 = \frac{a\mu}{\varepsilon\kappa - \nu}, \quad f_2 = \kappa - \nu, \quad g_1 = \frac{a(\kappa - \nu)}{\varepsilon\kappa - \nu}, \quad g_2 = \mu. \quad (6.80)$$

These formulas remain valid for  $n = 0$ ; in this case the terms containing  $L_{n-1}^{2\nu+1}(\xi)$  have to be taken to be zero. Thus we derive the representation for the radial functions (4.13) up to the constant  $B_n$ . The normalization condition (6.65) gives the value of this constant as

$$B_n = a\beta^{3/2} \sqrt{\frac{(\kappa - \nu)(\varepsilon\kappa - \nu)n!}{\mu\Gamma(n + 2\nu)}}. \quad (6.81)$$

This has been already verified in Section 4.5. Observe that Eq. (6.81) applies when  $n = 0$ .

The familiar recurrence relations for the Laguerre polynomials (8.5)–(8.6) allow to present the radial functions (4.13) in a traditional form [1], [16], [28] as

$$\begin{pmatrix} F(r) \\ G(r) \end{pmatrix} = a^2 \beta^{3/2} \sqrt{\frac{n!}{\mu(\kappa - \nu)(\varepsilon\kappa - \nu)\Gamma(n + 2\nu)}} \xi^{\nu-1} e^{-\xi/2}$$

$$\times \begin{pmatrix} \alpha_1 & \alpha_2 \\ \beta_1 & \beta_2 \end{pmatrix} \begin{pmatrix} L_{n-1}^{2\nu}(\xi) \\ L_n^{2\nu}(\xi) \end{pmatrix} \quad (6.82)$$

with

$$\alpha_1 = \sqrt{1+\varepsilon} \left( (\kappa - \nu) \sqrt{1+\varepsilon} + \mu \sqrt{1-\varepsilon} \right), \quad \alpha_2 = -\sqrt{1+\varepsilon} \left( (\kappa - \nu) \sqrt{1+\varepsilon} - \mu \sqrt{1-\varepsilon} \right), \quad (6.83)$$

$$\beta_1 = \sqrt{1-\varepsilon} \left( (\kappa - \nu) \sqrt{1+\varepsilon} + \mu \sqrt{1-\varepsilon} \right), \quad \beta_2 = \sqrt{1-\varepsilon} \left( (\kappa - \nu) \sqrt{1+\varepsilon} - \mu \sqrt{1-\varepsilon} \right). \quad (6.84)$$

By (8.2) one can rewrite this representation in terms of the confluent hypergeometric functions.

**6.4. Nonrelativistic Limit of the Wave Functions.** Throughout the paper we have always used the notation  $n = n_r$  for the radial quantum number, which determines the number of zeros of the radial functions in the relativistic Coulomb problem; see (4.13). For the sake of passing to the limit  $c \rightarrow \infty$  in this section, let us introduce the principal quantum number of the nonrelativistic hydrogen atom as  $n = n_r + |\kappa| = n_r + j + 1/2$  and temporarily consider  $N = n_r + \nu$  as its “relativistic analog”. As  $c \rightarrow \infty$  one gets

$$\nu = \sqrt{\kappa^2 - \mu^2} = |\kappa| - \frac{\mu^2}{2|\kappa|} - \frac{\mu^4}{8|\kappa|^3} + O(\mu^6), \quad (6.85)$$

$$N = n_r + \nu = n_r + |\kappa| - \frac{\mu^2}{2|\kappa|} - \frac{\mu^4}{8|\kappa|^3} + O(\mu^6) \quad (6.86)$$

as  $\mu = Ze^2/\hbar c \rightarrow 0$ . As a result, for the discrete energy levels

$$\varepsilon = \left( 1 + \frac{\mu^2}{N^2} \right)^{-1/2} \quad (6.87)$$

we arrive at the expansion (4.17) in the nonrelativistic limit  $c \rightarrow \infty$ .

In a similar fashion,

$$a = \sqrt{1 - \varepsilon^2} = \frac{\mu}{n_r + |\kappa|} \left( 1 + \frac{n_r \mu^2}{2|\kappa| (n_r + |\kappa|)^2} + O(\mu^4) \right), \quad (6.88)$$

$$\xi = \xi(c) = 2a \frac{mc}{\hbar} r = \frac{2Ze^2 m}{n\hbar^2} r (1 + O(\mu^2)) \quad (6.89)$$

as  $\mu \rightarrow 0$ , thus giving

$$\lim_{c \rightarrow \infty} \xi(c) = \eta = \frac{2Z}{n} \left( \frac{r}{a_0} \right) \quad (6.90)$$

by (3.3). Also

$$\kappa - \nu = (\kappa - |\kappa|) + \frac{\mu^2}{2|\kappa|} + O(\mu^4), \quad (6.91)$$

$$\varepsilon \kappa - \nu = (\kappa - |\kappa|) + \frac{(n_r + |\kappa|)^2 - \kappa |\kappa|}{2|\kappa| (n_r + |\kappa|)^2} \mu^2 + O(\mu^4) \quad (6.92)$$

as  $\mu \rightarrow 0$ . This allows to evaluate the nonrelativistic limit of the transition matrix:

$$S = \begin{pmatrix} f_1 & f_2 \\ g_1 & g_2 \end{pmatrix} = \begin{pmatrix} \frac{a\mu}{\varepsilon \kappa - \nu} & \kappa - \nu \\ \frac{a(\kappa - \nu)}{\varepsilon \kappa - \nu} & \mu \end{pmatrix}. \quad (6.93)$$

There are two distinct cases with the end result

$$\psi_{\pm} = \begin{pmatrix} \mathcal{Y}^{\pm} F \\ i\mathcal{Y}^{\mp} G \end{pmatrix} \rightarrow \begin{pmatrix} \pm \mathcal{Y}^{\pm} R \\ 0 \end{pmatrix}, \quad \mu \rightarrow 0. \quad (6.94)$$

Here  $R = R_{nl}(r)$  are the nonrelativistic radial functions (3.2)–(3.3) and  $\mathcal{Y}^{\pm} = \mathcal{Y}_{jm}^{(j \pm 1/2)}(\mathbf{n})$  are the spinor spherical harmonics (6.5).

Indeed, if  $\kappa = |\kappa| = j + 1/2 = l$ ,

$$S = S_+(\mu) = \begin{pmatrix} \frac{2\kappa(n_r + \kappa)}{n_r(n_r + 2\kappa)} + O(\mu^2) & \frac{\mu^2}{2|\kappa|} + O(\mu^4) \\ \frac{(n_r + \kappa)\mu}{n_r(n_r + 2\kappa)} + O(\mu^3) & \mu \end{pmatrix} \sim \begin{pmatrix} 1 & \mu^2 \\ \mu & \mu \end{pmatrix}$$

as  $\mu \rightarrow 0$  or

$$\lim_{\mu \rightarrow 0} S_+(\mu) = \frac{2nl}{n^2 - l^2} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}. \quad (6.95)$$

In this case  $\nu \rightarrow l$  and, therefore,

$$\begin{pmatrix} F(r) \\ G(r) \end{pmatrix} \rightarrow \left( \frac{Ze^2 m}{\hbar^2} \right)^{3/2} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \frac{2}{n^2} \sqrt{\frac{(n-l-1)!}{(n+l)!}} \eta^l e^{-\eta/2} \eta L_{n-l-1}^{2l+1}(\eta) \quad (6.96)$$

in the limit  $c \rightarrow \infty$  thus giving

$$\psi_+ = \begin{pmatrix} \mathcal{Y}^+ F \\ i\mathcal{Y}^- G \end{pmatrix} \rightarrow \begin{pmatrix} \mathcal{Y}^+ R \\ 0 \end{pmatrix}, \quad \mu \rightarrow 0. \quad (6.97)$$

In a similar fashion, when  $\kappa = -|\kappa| = -(j + 1/2) = -l - 1$  one gets

$$\psi_- = \begin{pmatrix} \mathcal{Y}^- F \\ i\mathcal{Y}^+ G \end{pmatrix} \rightarrow \begin{pmatrix} -\mathcal{Y}^- R \\ 0 \end{pmatrix}, \quad \mu \rightarrow 0 \quad (6.98)$$

due to the corresponding asymptotic form of the transition matrix  $S = S_-(\mu)$ :

$$S_-(\mu) = \begin{pmatrix} -\frac{\mu^2}{2|\kappa|(n_r + |\kappa|)} + O(\mu^4) & -2|\kappa| + O(\mu^2) \\ \frac{\mu}{n_r + |\kappa|} + O(\mu^3) & \mu \end{pmatrix} \sim \begin{pmatrix} \mu^2 & 1 \\ \mu & \mu \end{pmatrix} \quad (6.99)$$

as  $\mu \rightarrow 0$  [57]. This completes the proof of (6.94).

The representation of the radial functions in the form (4.13), due to Nikiforov and Uvarov [57], is well adapted for passing to the nonrelativistic limit since one coefficient of the transition matrix  $S$  is much larger than the others as  $\mu \rightarrow 0$ . In the traditional form (6.83)–(6.84), however, there is an overlap of the orders of these coefficients and one has to use the recurrence relations (8.5)–(8.6) in order to obtain the nonrelativistic wave functions as a limiting case of relativistic ones.

## 7. METHOD OF SEPARATION OF VARIABLES AND ITS EXTENSION

In this section we give an extension of the method of separation of variables, that is used in theoretical and mathematical physics for solving partial differential equations, from a single equation to a system of partial differential equations which we call Dirac-type system.

**7.1. Method of Separation of Variables.** We follow [57] and give an extension for suitable Dirac's systems. The method of separation of the variables helps to find particular solutions of equation

$$\mathcal{L}u = 0 \quad (7.1)$$

if the operator  $\mathcal{L}$  can be represented in the form

$$\mathcal{L} = \mathcal{M}_1\mathcal{N}_1 + \mathcal{M}_2\mathcal{N}_2. \quad (7.2)$$

Here the operators  $\mathcal{M}_1$  and  $\mathcal{M}_2$  act only on one subset of the variables, and the operators  $\mathcal{N}_1$  and  $\mathcal{N}_2$  act on the others; a product of operators  $\mathcal{M}_i\mathcal{N}_k$  means the result of applying them successively  $(\mathcal{M}_i\mathcal{N}_k)u = \mathcal{M}_i(\mathcal{N}_ku)$  with  $i, k = 1, 2$ ; it is assumed that the operators  $\mathcal{M}_i$  and  $\mathcal{N}_i$  are linear operators.

We look for solutions of equation (7.1) in the form

$$u = f g, \quad (7.3)$$

where the first unknown function  $f$  depends only on the first set of variables and the second function  $g$  depends on the others. Since

$$\begin{aligned} \mathcal{M}_i\mathcal{N}_ku &= (\mathcal{M}_i\mathcal{N}_k)(f g) = \mathcal{M}_i(\mathcal{N}_k(f g)) \\ &= \mathcal{M}_i(f (\mathcal{N}_kg)) = (\mathcal{M}_if)(\mathcal{N}_kg) \end{aligned}$$

the equation  $\mathcal{L}u = 0$  can be rewritten in the form

$$\frac{\mathcal{M}_1f}{\mathcal{M}_2f} = -\frac{\mathcal{N}_2g}{\mathcal{N}_1g},$$

where the left hand side is independent of the second group of the variables and the right hand side is independent of the first ones. Thus, we must have

$$\frac{\mathcal{M}_1f}{\mathcal{M}_2f} = -\frac{\mathcal{N}_2g}{\mathcal{N}_1g} = \lambda,$$

where  $\lambda$  is a constant, and one obtains equations

$$\mathcal{M}_1f = \lambda\mathcal{M}_2f, \quad \mathcal{N}_2g = -\lambda\mathcal{N}_1g \quad (7.4)$$

each containing functions of only some of the variables. Since  $\mathcal{L}$  is linear, a linear combination of solutions,

$$u = \sum_k c_k f_k g_k \quad (7.5)$$

with some constants  $c_k$ , corresponding to all admissible values of  $\lambda = \lambda_k$ , will be a solution of the original equation (7.1). Under certain condition of the completeness of the constructed set of particular solutions, every solution of (7.1) can be represented in the form (7.5). The method of separation of variables is very useful in theoretical and mathematical physics and partial differential equations — including solutions of the nonrelativistic Schrödinger equation — but, as we have seen in Section 6.2, it should be modified in the case of the Dirac equation.

**Example.** The Schrödinger equation in the central field with the potential energy  $U(r)$  is

$$\Delta\psi + \frac{2m}{\hbar^2} (E - U(r)) \psi = 0. \quad (7.6)$$

The Laplace operator in the spherical coordinates  $r, \theta, \varphi$  has the form [55], [57]

$$\Delta = \Delta_r + \frac{1}{r^2} \Delta_\omega \quad (7.7)$$

with

$$\Delta_r = \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right), \quad \Delta_\omega = \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \varphi^2}. \quad (7.8)$$

Thus

$$\mathcal{M}_1 = \Delta_r + \frac{2m}{\hbar^2} (E - U(r)), \quad \mathcal{M}_2 = \frac{1}{r^2} \quad (7.9)$$

$$\mathcal{N}_1 = \text{id} = I, \quad \mathcal{N}_2 = \Delta_\omega \quad (7.10)$$

and separation of the variables  $\psi = R(r) Y(\theta, \varphi)$  gives

$$\Delta_\omega Y(\theta, \varphi) + \lambda Y(\theta, \varphi) = 0, \quad (7.11)$$

$$\frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{dR(r)}{dr} \right) + \left( \frac{2m}{\hbar^2} (E - U(r)) - \frac{\lambda}{r^2} \right) R(r) = 0. \quad (7.12)$$

Bounded single-valued solutions of equation (7.11) on the sphere  $S^2$  exist only when  $\lambda = l(l+1)$  with  $l = 0, 1, 2, \dots$ . They are the spherical harmonics  $Y = Y_{lm}(\theta, \varphi)$ .

**7.2. Dirac-Type Systems.** Let us consider the system of two equations

$$\mathcal{P}u = \alpha v, \quad (7.13)$$

$$\mathcal{P}v = \beta u, \quad (7.14)$$

where  $u = u(\mathbf{x})$  and  $v = v(\mathbf{x})$  are some unknown (complex) vector valued functions on  $\mathbf{R}^n$  (or  $\mathbf{C}^n$ ). Here operator  $\mathcal{P}$  has the following structure

$$\mathcal{P} = \mathcal{N}(\mathbf{n}) (\mathcal{D}_1(r) \mathcal{L}_1(\mathbf{n}) + \mathcal{D}_2(r) \mathcal{L}_2(\mathbf{n})), \quad \mathcal{N}^2(\mathbf{n}) = \text{id} = I, \quad (7.15)$$

where  $\mathcal{D}_i = \mathcal{D}_i(r)$ ,  $\mathcal{L}_k = \mathcal{L}_k(\mathbf{n})$  and  $\mathcal{N} = \mathcal{N}(\mathbf{n})$  are linear operators acting with respect to two different subsets of variables, say “radial”  $r$  and “angular”  $\mathbf{n}$  variables, respectively (in the case of the hyperspherical coordinates in  $\mathbf{R}^n$  [55] one gets  $\mathbf{x} = r\mathbf{n}$  and  $\mathbf{n}^2 = 1$ , which justifies our terminology). The following algebraic properties hold

$$[\mathcal{D}_i, \mathcal{L}_k] = [\mathcal{D}_i, \mathcal{N}] = 0, \quad (7.16)$$

$$[\mathcal{N}, \mathcal{L}_1] = [\mathcal{L}_1, \mathcal{L}_2] = 0, \quad (7.17)$$

$$\mathcal{N}\mathcal{L}_2 + \mathcal{L}_2\mathcal{N} = \gamma\mathcal{N}, \quad (7.18)$$

where  $[\mathcal{A}, \mathcal{B}] = \mathcal{A}\mathcal{B} - \mathcal{B}\mathcal{A}$  is the commutator and  $\gamma$  is some constant.

We look for solutions of (7.13)–(7.14) in the form

$$u = \mathcal{Y}(\mathbf{n}) R(r), \quad (7.19)$$

$$v = (\mathcal{N}\mathcal{Y}(\mathbf{n})) S(r), \quad (7.20)$$

where  $\mathcal{Y}$  is the common eigenfunction of commuting operators  $\mathcal{L}_1$  and  $\mathcal{L}_2$ :

$$\mathcal{L}_1\mathcal{Y} = \kappa_1\mathcal{Y}, \quad \mathcal{L}_2\mathcal{Y} = \kappa_2\mathcal{Y}. \quad (7.21)$$

If  $w = w(\mathbf{x}) = F(\mathbf{n})G(r)$ , we define the action of the “radial” and “angular” operators in (7.15) as follows

$$\mathcal{L}_i w = (\mathcal{L}_i F)G, \quad \mathcal{N}w = (\mathcal{N}F)G, \quad \mathcal{D}_k w = F(\mathcal{D}_k G). \quad (7.22)$$

The Ansatz (7.19)–(7.20) results in two equations for our “radial” functions  $R$  and  $S$ :

$$\kappa_1 \mathcal{D}_1 R + \kappa_2 \mathcal{D}_2 R = \alpha S, \quad (7.23)$$

$$\kappa_1 \mathcal{D}_1 S + (\gamma - \kappa_2) \mathcal{D}_2 S = \beta R. \quad (7.24)$$

Indeed, in view of (7.13)–(7.14) and (7.19)–(7.21) one gets

$$\begin{aligned} \mathcal{P}u &= \mathcal{N}(\mathcal{D}_1 \mathcal{L}_1 + \mathcal{D}_2 \mathcal{L}_2) \mathcal{Y}R \\ &= \mathcal{N}((\mathcal{L}_1 \mathcal{Y})(\mathcal{D}_1 R) + (\mathcal{L}_2 \mathcal{Y})(\mathcal{D}_2 R)) \\ &= (\mathcal{N} \mathcal{Y})(\kappa_1 \mathcal{D}_1 R + \kappa_2 \mathcal{D}_2 R) \\ &= \alpha (\mathcal{N} \mathcal{Y}) S = \alpha v, \end{aligned}$$

which gives (7.23). In a similar fashion, with the aid of (7.18)

$$\begin{aligned} \mathcal{P}v &= \mathcal{N}(\mathcal{D}_1 \mathcal{L}_1 + \mathcal{D}_2 \mathcal{L}_2) (\mathcal{N} \mathcal{Y}) S \\ &= \mathcal{N}((\mathcal{L}_1 \mathcal{N} \mathcal{Y})(\mathcal{D}_1 S) + (\mathcal{L}_2 \mathcal{N} \mathcal{Y})(\mathcal{D}_2 S)) \\ &= (\mathcal{N} \mathcal{L}_1 \mathcal{N} \mathcal{Y})(\mathcal{D}_1 S) + (\mathcal{N} \mathcal{L}_2 \mathcal{N} \mathcal{Y})(\mathcal{D}_2 S) \\ &= (\mathcal{N}^2 \mathcal{L}_1 \mathcal{Y})(\mathcal{D}_1 S) + ((\gamma - \mathcal{L}_2) \mathcal{N}^2 \mathcal{Y})(\mathcal{D}_2 S) \\ &= \mathcal{Y}(\kappa_1 \mathcal{D}_1 S + (\gamma - \kappa_2) \mathcal{D}_2 S) = \beta \mathcal{Y}R = \beta u, \end{aligned}$$

which results in the second equation (7.24) and our proof is complete.

**Example.** The original Dirac system (6.22)–(6.23) has

$$\psi = \begin{pmatrix} \mathbf{u} \\ \mathbf{v} \end{pmatrix} = \begin{pmatrix} \boldsymbol{\varphi} \\ \boldsymbol{\chi} \end{pmatrix}$$

and

$$\mathcal{P} = c\boldsymbol{\sigma}\mathbf{p} = \hbar c(\boldsymbol{\sigma}\mathbf{n}) \left( \frac{1}{i} \frac{\partial}{\partial r} + \frac{i}{r} \boldsymbol{\sigma}\mathbf{l} \right). \quad (7.25)$$

Here

$$\mathcal{N} = \boldsymbol{\sigma}\mathbf{n}, \quad \mathcal{D}_1 = \frac{\hbar c}{i} \frac{\partial}{\partial r}, \quad \mathcal{L}_1 = \text{id} = I, \quad \mathcal{D}_2 = \frac{i\hbar c}{r}, \quad \mathcal{L}_2 = \boldsymbol{\sigma}\mathbf{l} \quad (7.26)$$

and

$$\alpha(r) = E + mc^2 - U(r), \quad \beta(r) = E - mc^2 - U(r), \quad \gamma = -2 \quad (7.27)$$

by (6.28). Moreover,  $\kappa_1 = 1$ ,  $\kappa_2 = -(1 + \kappa)$  and we use  $R = F(r)$ ,  $S = -iG(r)$ . The Ansatz (6.29)–(6.30) gives the familiar radial equations (6.31)–(6.32).

## 8. APPENDIX: USEFUL FORMULAS

This section contains some relations involving the generalized hypergeometric series, the Laguerre and Hahn polynomials, the spherical harmonics and Clebsch–Gordan coefficients, which are used throughout the paper.

The generalized hypergeometric series is [3], [10], [22], [42]

$${}_pF_q(a_1, a_2, \dots, a_p; b_1, b_2, \dots, b_q; z) \quad (8.1)$$



$$= {}_pF_q \left( \begin{matrix} a_1, a_2, \dots, a_p \\ b_1, b_2, \dots, b_q \end{matrix} ; z \right) = \sum_{n=0}^{\infty} \frac{(a_1)_n (a_2)_n \dots (a_p)_n}{(b_1)_n (b_2)_n \dots (b_q)_n} \frac{z^n}{n!},$$

where  $(a)_n = a(a+1)\dots(a+n-1) = \Gamma(a+n)/\Gamma(a)$ . By the ratio test, the  ${}_pF_q$  series converges absolutely for all complex values of  $z$  if  $p \leq q$ , and for  $|z| < 1$  if  $p = q+1$ . By an extension of the ratio test ([24], p. 241), it converges absolutely for  $|z| = 1$  if  $p = q+1$  and  $z \neq 0$  or  $p = q+1$  and  $\operatorname{Re}[b_1 + \dots + b_q - (a_1 + \dots + a_p)] > 0$ . If  $p > q+1$  and  $z \neq 0$  or  $p = q+1$  and  $|z| > 1$ , then this series diverges, unless it terminates.

The Laguerre polynomials are defined as [3], [55], [57], [74]

$$L_n^\alpha(x) = \frac{\Gamma(\alpha+n+1)}{n! \Gamma(\alpha+1)} {}_1F_1 \left( \begin{matrix} -n \\ \alpha+1 \end{matrix} ; x \right). \quad (8.2)$$

It is a consequence of Theorem 3. The differentiation formulas [55], [57]

$$\frac{d}{dx} L_n^\alpha(x) = -L_{n-1}^{\alpha+1}(x), \quad (8.3)$$

$$x \frac{d}{dx} L_n^\alpha(x) = n L_n^\alpha(x) - (\alpha+n) L_{n-1}^\alpha(x) \quad (8.4)$$

imply a recurrence relation

$$x L_{n-1}^{\alpha+1}(x) = (\alpha+n) L_{n-1}^\alpha(x) - n L_n^\alpha(x). \quad (8.5)$$

The simplest case of the connecting relation (2.12) is

$$L_n^\alpha(x) = L_n^{\alpha+1}(x) - L_{n-1}^{\alpha+1}(x). \quad (8.6)$$

The Hahn polynomials are [55], [57]

$$h_n^{(\alpha, \beta)}(x, N) = (-1)^n \frac{\Gamma(N)(\beta+1)_n}{n! \Gamma(N-n)} {}_3F_2 \left( \begin{matrix} -n, \alpha+\beta+n+1, -x \\ \beta+1, 1-N \end{matrix} ; 1 \right). \quad (8.7)$$

We usually omit the argument of the hypergeometric series  ${}_3F_2$  if it is equal to one. An asymptotic relation with the Jacobi polynomials is

$$\frac{1}{\tilde{N}^n} h_n^{(\alpha, \beta)} \left( \frac{\tilde{N}}{2} (1+s) - \frac{\beta+1}{2}, N \right) = P_n^{(\alpha, \beta)}(s) + O\left(\frac{1}{\tilde{N}^2}\right), \quad (8.8)$$

where  $\tilde{N} = N + (\alpha + \beta)/2$  and  $N \rightarrow \infty$ ; see [55] for more details.

Thomae's transformation [10], [42] is

$${}_3F_2 \left( \begin{matrix} -n, a, b \\ c, d \end{matrix} ; 1 \right) = \frac{(d-b)_n}{(d)_n} {}_3F_2 \left( \begin{matrix} -n, c-a, b \\ c, b-d-n+1 \end{matrix} ; 1 \right) \quad (8.9)$$

with  $n = 0, 1, 2, \dots$ .

The summation formula of Gauss [3], [10], [42]

$${}_2F_1 \left( \begin{matrix} a, b \\ c \end{matrix} ; 1 \right) = \frac{\Gamma(c) \Gamma(c-a-b)}{\Gamma(c-a) \Gamma(c-b)}, \quad \operatorname{Re}(c-a-b) > 0. \quad (8.10)$$

The gamma function is defined as [3], [36], [57]

$$\Gamma(z) = \int_0^\infty e^{-t} t^{z-1} dt, \quad \operatorname{Re} z > 0. \quad (8.11)$$

It can be continued analytically over the whole complex plane except the points  $z = 0, -1, -2, \dots$  at which it has simple poles. Functional equations are

$$\Gamma(z+1) = z\Gamma(z), \quad (8.12)$$

$$\Gamma(z)\Gamma(1-z) = \frac{\pi}{\sin \pi z}, \quad (8.13)$$

$$2^{2z-1}\Gamma(z)\Gamma(z+1/2) = \sqrt{\pi}\Gamma(2z). \quad (8.14)$$

The generating function for the Legendre polynomials and the addition theorem for spherical harmonics give rise to the following expansion formula [57], [80]

$$\frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} = \sum_{l=0}^{\infty} \sum_{m=-l}^l \frac{4\pi}{2l+1} \frac{r_{<}^l}{r_{>}^{l+1}} Y_{lm}(\theta_1, \varphi_1) Y_{lm}^*(\theta_2, \varphi_2), \quad (8.15)$$

where  $r_{<} = \min(r_1, r_2)$  and  $r_{>} = \max(r_1, r_2)$ .

The Clebsch–Gordan series for the spherical harmonics is [55], [63], [80]

$$\begin{aligned} Y_{l_1 m_1}(\theta, \varphi) Y_{l_2 m_2}(\theta, \varphi) &= \sum_{l=|l_1-l_2|}^{l_1+l_2} \sqrt{\frac{(2l_1+1)(2l_2+1)}{4\pi(2l+1)}} \\ &\quad \times C_{l_1 m_1 l_2 m_2}^{l, m_1+m_2} C_{l_1 0 l_2 0}^{l, 0} Y_{l, m_1+m_2}(\theta, \varphi), \end{aligned} \quad (8.16)$$

where  $C_{l_1 m_1 l_2 m_2}^{lm}$  are the Clebsch–Gordan coefficients. The special case  $l_2 = 1$  reads [39]

$$-\sin \theta e^{i\varphi} Y_{l, m-1} = \sqrt{\frac{(l+m)(l+m+1)}{(2l+1)(2l+3)}} Y_{l+1, m} - \sqrt{\frac{(l-m)(l-m-1)}{(2l+1)(2l-1)}} Y_{l-1, m}, \quad (8.17)$$

$$\sin \theta e^{-i\varphi} Y_{l, m+1} = \sqrt{\frac{(l-m)(l-m+1)}{(2l+1)(2l+3)}} Y_{l+1, m} - \sqrt{\frac{(l+m)(l+m+1)}{(2l+1)(2l-1)}} Y_{l-1, m}, \quad (8.18)$$

$$\cos \theta Y_{lm} = \sqrt{\frac{(l+1)^2 - m^2}{(2l+1)(2l+3)}} Y_{l+1, m} + \sqrt{\frac{l^2 - m^2}{(2l-1)(2l+1)}} Y_{l-1, m}, \quad (8.19)$$

where

$$\sqrt{\frac{8\pi}{3}} Y_{1, \pm 1} = \mp \sin \theta e^{\pm i\varphi}, \quad \sqrt{\frac{4\pi}{3}} Y_{10} = \cos \theta. \quad (8.20)$$

These relations allow to prove (6.14) by a direct calculation.

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DEPARTMENT OF MATHEMATICS AND STATISTICS, ARIZONA STATE UNIVERSITY, TEMPE, AZ 85287, U.S.A.

*E-mail address:* `sks@asu.edu`

*URL:* `http://hahn.la.asu.edu/~suslov/index.html`

DEPARTMENT OF PHYSICS AND ASTRONOMY, UNIVERSITY OF HAWAII AT MANOA, 2505 CORREA RD., HONOLULU, HAWAII 96822, U.S.A.

*E-mail address:* `btrey@hawaii.edu`